On the Ground State Energy of Large Coulomb Systems

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Zusammenfassung

In dieser Doktorarbeit werden zwei verschiedene Coulomb-Systeme im Vielteilchen-Limes betrachtet. Zuerst wird das Tröpfchenmodell für die Wechselwirkung von Nukleonen mit einem Hintergrund von Elektronen untersucht. Dabei wird der Grenzwert betrachtet bei dem das Verhältnis der Elektronen- zur Neukleonenladungsdichte klein ist. In drei Dimensionen wird gezeigt, dass der thermodynamische Limes der Grundzustandsenergie zur führenden Ordnung der eines einzelnen Atomkernes entspricht wenn die Ladungsdichte klein ist. In zwei Dimensionen wird der Koeffizient der führenden Ordnung hergeleitet und es werden Fehlerschranken bewiesen, die die Größenordnung einer vermuteten Asymptotik der zweiten Ordnung haben. Außerdem wird ein Resultat bewiesen zur gleichmäßigen Verteilung der Energie im Raum mithilfe einer Methode, die Armstrong und Serfaty verwendeten um die gleichmäßige Verteilung der Energie im Jellium Modell zu beweisen.

Das zweite Coulomb-System behandelt viele Polaronen in der Pekar-Tomasevich Näherung. Benguria, Frank und Lieb bewiesen 2015, dass die entsprechende Grundzustandsenergie propotional ist zu $-N^{7/5}$ für große N. Sie bewiesen eine obere Schranke für den Koeffizienten und formulierten die Vermutung, dass diese scharf ist. In dieser Doktorarbeit wird bewiesen, dass die Vermutung korrekt ist indem die entsprechende untere Schranke hergleitet wird. Dabei wird ein geladenes Bose-Gas mit Coulomb-Wechselwirkung und einem Hintergrund entgegengesetzter Ladung betrachtet. Mithilfe von Methoden von Lieb und Solovej kann Bogolubov Theorie verwendet werden.

Abstract

This thesis is concerned with two different Coulomb systems in the many-particle limit. First of all, the liquid drop model for nuclei interacting with a neutralizing homogeneous background of electrons is considered. The regime that is of interest is when the fraction between the electron and the nucleon charge density is small. In three dimensions, it is shown that in this dilute limit the thermodynamic ground state energy is given to leading order by that of an isolated nucleus. In two dimensions, it is proven how the leading order coefficient of the thermodynamic ground state energy is in the dilute limit and error estimates are shown that reproduce the second order of a conjectured asymptotics. Furthermore, a result is derived on the uniform distribution of energy in any dimension which is based on a method Armstrong and Serfaty used to prove uniform distribution of energy for the jellium model.

The second Coulomb system that is considered is the "neutral" case of the many-polaron system in the Pekar-Tomasevich approximation. In 2015, Benguria, Frank and Lieb showed that in this case the ground state energy goes as $-N^{7/5}$ for large N. They proved an upper bound for the coefficient and conjectured it to be the correct one. Here, it is established that this is indeed true by proving the corresponding lower bound. To do so, a one-component charged Bose gas with Coulomb interaction and a background with variable charge distribution is studied. Adapting methods of Lieb and Solovej one can justify Bogolubov theory for this model.

Chapter 1

Introduction and Main Theorems

1.1 General Introduction

One of the most astonishing facts about nature is that it can be so precisely described in terms of mathematics. Whether it is Newton's mechanics describing the basics of how we experience masses moving, accelerating or resting in every day life. Or whether it is Maxwell's equations describing electromagnetism. Even the behavior of the smallest particles we currently know can be described using rigorous mathematics. Well, at least some of the description is rigorous.

There are four known interactions in nature. [44] The interaction with the smallest coupling constant is gravity. Since this interaction is so weak it has the largest bound states, namely us living on earth or our solar system within our galaxy. At the same time, there is only one type of mass. So there is no neutrality which is why gravity can reach arbitrarily far.

The strongest interaction that is currently known is - as the name says - the strong interaction. Because of this, it has the smallest bound states, for example protons and neutrons within an atomic nucleus.

The interaction which is not as strong as the strong interaction but still much stronger than gravity is electromagnetism. This is why it has bound states which are much larger than protons or neutrons within an atomic nucleus, but still much smaller than the bound states of gravity. For example matter as we experience it in everyday life is a bound state of the electromagnetic interaction. Or, much simpler of course, molecules as well.

This thesis is concerned with large systems with Coulomb interaction, i.e. purely electrostatics. There are two kinds of electric charges, positive and negative ones. The strength of the Coulomb interaction therefore enforces neutrality resulting in a far field which decays much faster than the Coulomb field of one type of charge itself.

Why do we do mathematics? Apart from physics and natural sciences there are many applications of mathematics like engineering. However, one might suggest that it is interesting to study mathematics in and of itself. Just as people have always been wanting to explore the earth as one can experience it, from sailors in the sixteens century to physicists colliding high energy particles in the 20th century, apart from many other reasons also just out of curiosity, so one might be interested in the a priori world of mathematics for its own sake apart from all applications that it has and will have in the future.

The area of mathematics that this thesis is concerned with is analysis. Roughly put it presupposes an a priori understanding of space (and maybe also of time) and than studies what one might be able to say about definitions on this space.

Maxwell equations In the second half of the nineteenth century Maxwell formulated his theory of the electromagnetic interaction [45, p. 310]. A charge distribution $f : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}$ where $(x, t) \in \mathbb{R}^3 \times \mathbb{R}$ denotes a position in space x at time t induces an electric field $\mathbf{E} \in C^1(\mathbb{R}^3 \times \mathbb{R}, \mathbb{R}^3)$ and a magnetic field $\mathbf{B} \in C^1(\mathbb{R}^3 \times \mathbb{R}, \mathbb{R}^3)$ such that the system of partial differential equations is fulfilled [45, p. 314] in suitable units

$$\nabla \mathbf{E} = f, \qquad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t},$$
$$\nabla \mathbf{B} = 0, \qquad \nabla \times \mathbf{B} = \frac{\partial \mathbf{E}}{\partial t} + \mathbf{j}.$$

Here, $\mathbf{j}$ denotes the electric current that fulfills $\nabla \mathbf{j} + \frac{\partial f}{\partial t} = 0$ and it is assumed that the electric polarization and the magnetization is zero. One observes that a magnetic field that changes with time induces a rotational electric field and an electric field that changes with time induces a rotational magnetic field. This is the mathematical description of electromagnetic waves. Furthermore, the fact that the divergence of the magnetic field vanishes implies that there are no magnetic monopoles.

In this thesis Coulomb systems are considered. So the charge distribution f is not dependent on time, the electric current is zero and there are no rotational fields, neither electric nor magnetic. This is why one can describe $\mathbf{E}$ in terms of a potential $v \in C^2(\mathbb{R}^3, \mathbb{R})$ such that $-\boldsymbol{\nabla} v = c_d \mathbf{E}$. The resulting partial differential equation depending on the static charge density f and the potential v can be formulated in any dimension $d \in \mathbb{N}$ (let $d \geq 2$). It is the Poisson equation

$$\begin{cases} -\Delta v = c_d f \text{ in } \mathbb{R}^d, \\ \quad v \in H^1(\mathbb{R}^d), \end{cases}$$

where $c_2 := 2\pi$ and $c_d := (d-2)|\mathbb{S}^{d-1}|$ with the $d-1$ dimensional unit sphere $\mathbb{S}^{d-1}$. For $Q \subseteq \mathbb{R}^d$, $H^1(Q)$ denotes the Sobolev space of functions in the Lebesgue space $L^2(Q)$ that have weak derivatives which are in $L^2(Q)$. One solution can be expressed in terms of the fundamental solution of the Laplacian

$$v(x) := \int_{\mathbb{R}^d} G(x-y) f(y) \, \mathrm{d}y \,,$$

for $x \in \mathbb{R}^d$, where $G(x) := \ln \frac{1}{|x|}$ for $d = 2$ and $G(x) := \frac{1}{|x|^{d-2}}$ for $d \geq 3$.

Outline of this thesis In Chapters 2 and 3 the liquid drop model is considered in a cube $Q_L := (-L/2, L/2)^d$ with a charge distribution $1_{\Omega_{\rho,L}}$ for $\Omega_{\rho,L} \subset Q_L$ and a constant background $\rho 1_{Q_L}$ where $\rho \in (0,1)$ and $|\Omega| = \rho L^d$. The energy in d dimensions with whole space boundary condition is

$$\mathcal{E}_{\rho,L}(\Omega_{\rho,L}) := \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L}\int_{Q_L} (1_{\Omega_{\rho,L}}(x) - \rho) G(x-y)(1_{\Omega_{\rho,L}}(y) - \rho)\,\mathrm{d}x\,\mathrm{d}y\,, \qquad (1.1)$$

where $G(x) := \frac{1}{|x|^{d-2}}$ for $d \geq 3$ and $G(x) := \ln \frac{1}{|x|}$ for $d = 2$. Note that when subsets of $\mathbb{R}^d$ are considered they are always assumed to be Lebesgue measurable.

In the following sections a more detailed motivation for this model is given. For now, just note that there is an attractive short range term, the perimeter, and a repulsive long-range term, the Coulomb energy of the system (see e.g. [32, 1, 25]). This thesis is concerned with estimating the corresponding ground state energy

$$E_{\rho,L} := \inf\Big\{\mathcal{E}_{\rho,L}(\Omega) : \Omega \subset Q_L, |\Omega| = \rho L^d\Big\}. \qquad (1.2)$$

In Chapter 2 the leading order for small densities $\rho > 0$ of the ground state energy is derived in dimension $d = 3$ with explicit error estimates depending on the size of the whole system L and the charge density of the background $\rho \in (0, \frac{1}{2})$. It is assumed $L \gg \frac{1}{\rho}$. This corresponds to first taking the thermodynamic limit $L \to \infty$ and then, the dilute limit $\rho \to 0$. Note that these limits are taken separately. The challenge is that one does not know whether the minimizer of the whole space problem is a ball.

In Chapter 3 further results on the liquid drop model are derived. First of all, the ground state energy is considered in dimension $d = 2$. As one would expect the problem is easier to solve than the three dimensional one. This is why the leading order of the limit $\rho \to 0$ of the ground state energy is deduced as well as error estimates that reproduce the order of a conjectured second order asymptotics. The proof gives insight into how connected components (droplets) of a minimizer look like.

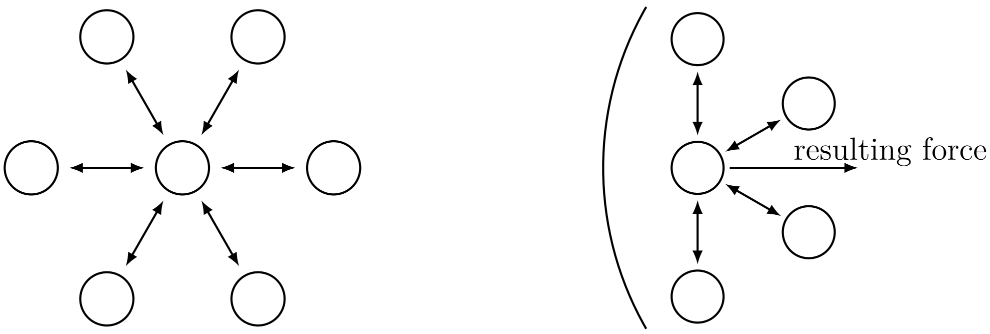
If one sets $f = 1_{\Omega_{\rho,L}} - \rho 1_{Q_L}$ and integrates by parts, the energy can be written in terms of the potential v

$$\begin{aligned}\mathcal{E}_{\rho,L}(\Omega_{\rho,L}) &= \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2c_d}\int_{\mathbb{R}^d} (-\Delta v) v \,\mathrm{d}x \\ &= \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2c_d}\int_{\mathbb{R}^d} |\nabla v|^2 \,\mathrm{d}x\,.\end{aligned}$$

In the second part of Chapter 3 a result on the uniform distribution of energy is derived for $d \geq 2$ on smaller scales $R \in \mathbb{R}$ with $1 \ll R \leq L$. The local energy considered is

$$\mathrm{Per}(\Omega_{\rho,L} \cap Q_R(a)) + \frac{1}{2}\int_{Q_R(a)} |\nabla v|^2 \,\mathrm{d}x\,,$$

where $Q_R(a) := a + Q_R$. Note that a different scaling is used in this case without the factor c_d^{-1}. The proof follows an approach that Armstrong and Serfarty used to prove uniform distribution of energy for the jellium model [2].



(a) On the inside the nuclear force of the surrounding nucleons cancels.

(b) Close to the boundary there is an effective force to the inside.

Figure 1.1: Nuclear force between the nucleons.

In Chapter 4 a completely different Coulomb system is considered. To prove a lower bound on a large polaron system the energy is linearized. This leads to the energy of a one component charged Bose gas taking the infimum over all possible background distributions of opposite charge. It is estimated similar to Lieb and Solovejs work on the one and two component charged Bose gases by Bogolubov theory [36, 37].

In the following sections a more detailed introduction to these chapters is given and the main theorems of this thesis are stated. For Chapter 4 some basic concepts of mathematical quantum mechanics are reviewed.

1.2 The three dimensional Liquid Drop Model

Chapter 2 on the three dimensional liquid drop model has been published in [13] as joined work with Rupert Frank and Tobias König.

An atomic nucleus consists of protons and neutrons. While protons have a positive electric charge, neutrons are – as the name suggests – electroneutral. What keeps the nucleons together is the nuclear force which is attractive but short ranged. It can be described by the Yukawa potential [44, p. 518]

$$Y_\omega(r) = \frac{C}{r} e^{-\omega r}$$

and it is effectively a nearest neighbor interaction. Inside of the nucleus the nuclear force of the surrounding nucleons cancels. So effectively there is no nuclear force inside of the nucleus. (See figure 1.1a.) On the boundary, however, the nuclear force of the surrounding nucleons does not cancel. So any nucleon on the boundary experiences a resulting force directed to the inside of the nucleus. This is why the nuclear force can be modeled as a surface tension. (See figure 1.1b.)

Liquid Drop Model without background Gamow's Liquid Drop Model [23] describes an atomic nucleus in terms of an incompressible, charged liquid. It has recently attracted a lot of attention in mathematics, see, for instance, [9, 10, 6, 29, 31, 39, 16, 32, 8, 30, 17].

The energy of this simple model in nuclear physics consists of a surface tension which is described by the perimeter term and an interaction which is described by the Coulomb term. First of all, consider a single nucleus without background. Possible shapes of this nucleus are (measurable) sets $\Omega \subset \mathbb{R}^3$ and their measure $|\Omega|$ is interpreted as the number of nucleons in suitable units. The energy of such a nucleus is, again in suitable units,

$$\mathcal{E}_0(\Omega) := \operatorname{Per}(\Omega) + \frac{1}{2}\int_\Omega \int_\Omega \frac{1}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y\,, \tag{1.3}$$

where $\operatorname{Per}(\Omega)$ denotes the perimeter in the sense of De Giorgi

$$\operatorname{Per}(\Omega) := \sup\left\{\int_\Omega \nabla\mathbf{F}\,\mathrm{d}x : \mathbf{F} \in C^1_\mathrm{c}(\mathbb{R}^3,\mathbb{R}^3), |\mathbf{F}| \le 1\right\},$$

(e.g. [15]). This leads to the variational problem of finding, for a given $A > 0$,

$$E_0(A) := \inf\{\mathcal{E}_0(\Omega) : \Omega \subset \mathbb{R}^3, |\Omega| = A\} \tag{1.4}$$

and $e_0 := \inf_{A>0} \frac{E_0(A)}{A}$.

It is known [16] (see also [32]) that there is an $A^* > 0$ such that $e_0 = \frac{E_0(A^*)}{A^*}$ and that there is a minimizing set $\Omega^* \subset \mathbb{R}^3$ with $|\Omega^*| = A^*$ such that $E_0(A^*) = \mathcal{E}_0(\Omega^*)$. This set Ω^* is strongly conjectured, but not known, to be a ball. Physically, it corresponds to a nucleus with the greatest binding energy per nucleon, which is a certain isotope of nickel.

The perimeter term favors Ω to be concentrated at one point. It is optimized by a ball (for a given nucleon number $|\Omega| = A > 0$). In contrast, the Coulomb energy is maximal for a ball. Since the perimeter term is heuristically proportional to $\sqrt{A}$ and the Coulomb term to A^2 the perimeter term dominates for small $A > 0$. This is why, for small $A > 0$ the minimizer of $\mathcal{E}_0$ is a ball [31]. It is conjectured in [10] that there is an $A_1 > 0$ such that a minimizer of $\mathcal{E}_0$ exists and is a ball for any nucleon number A with $0 < A \le A_1$ and such that there is no minimizer for $A > A_1$. Furthermore, it is conjectured that A_1 fulfills $\mathcal{E}_0(\Omega_1) = 2\mathcal{E}_0(\Omega_1/2^{1/3})$. So one ball Ω_1 with $|\Omega_1| = A_1$ has two times the energy of a ball with mass $A_1/2$. In [15] Frank, Killip and Nam prove the nonexistence for $A > 8$. (See Section 2 in [32] for an overview of the results.)

In the construction of the competitor set Ω that is used to prove the upper bound copies of a ball are placed on a lattice and than it is shown how the proof has to be modified if the minimizer of $\mathcal{E}_0$ is not a ball.

Liquid Drop Model with background The Coulomb force is very long ranged. Since the Coulomb potential $1/r$ is not integrable at infinity, local neutrality is needed to consider macroscopic systems. In nuclear matter it is a sea of delocalized electrons which provides a background of opposite charge. Therefore, a background density $\rho \in (0,1)$ is introduced and the system is considered inside a cube $Q_L = (-L/2, L/2)^3$ with $L > 0$.

The three dimensional energy functional is

$$\mathcal{E}_{\rho,L}(\Omega_{\rho,L}) = \operatorname{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L}\int_{Q_L} (1_{\Omega_{\rho,L}}(x) - \rho)\frac{1}{|x-y|}(1_{\Omega_{\rho,L}}(y) - \rho)\,\mathrm{d}x\,\mathrm{d}y\,. \tag{1.5}$$

Here, $\Omega_{\rho,L} \subset Q_L$ is assumed to be a neutral configuration, that is $|\Omega_{\rho,L}| = \rho L^3$. The goal will be to derive the leading order of the ground state energy

$$E_{\rho,L} = \inf\{\mathcal{E}_{\rho,L}(\Omega) : \Omega \subset Q_L, |\Omega| = \rho L^3\} \tag{1.6}$$

in the dilute limit $\rho \to 0$.

The main result of Chapter 2 is the following theorem on the behavior for small $\rho > 0$ of the thermodynamic limit of the energy $E_{\rho,L}$. It is proven for whole space boundary conditions. However, in Chapter 3, Theorem 3.22, it is deduced that the thermodynamic limit exists and is equal for Dirchlet, whole space, periodic and Neumann boundary conditions.

Theorem 1.1. *Let $\# \in \{\mathrm{Dir}, \infty, \mathrm{Per}, \mathrm{Neu}\}$ and $\rho \in (0, \frac{1}{2}]$. Then, the thermodynamic limit of the ground state energy for $d = 3$ is given by*

$$\lim_{L\to\infty} \frac{1}{L^3} E^{\#}_{\rho,L} = \frac{E_0(A^*)}{A^*}\rho + o(\rho) \quad \text{as } \rho \to 0. \tag{1.7}$$

In particular, it is equal for these boundary conditions

Remark 1.2. This result also holds for any boundary condition such that the potential $v_{\rho,L}$ of the minimizer $\Omega_{\rho,L}$ fulfills $\int_{\partial Q_L} v_{\rho,L}\nu \cdot \nabla v_{\rho,L}\,\mathrm{d}x' \leq 0$ for all $L > C$ and $\rho \in (0, \frac{1}{2}]$.

The leading order energy in the dilute limit comes from the energy of each droplet. The interaction of different droplets, the interaction of droplets with the background and the interaction of the background with the background only contribute to the energy at higher order. In particular, this means that the nucleon number A of each connected component is relevant for the leading order. The question of how droplets are arranged and whether they are arranged in terms of a lattice or not is not relevant for the leading order.

[1]The conjecture that for small ρ a minimizer is given by a periodic arrangement of nearly spherical droplets guides the proof of the upper bound. Since the arrangement of the droplets does not contribute to the leading order evaluating the energy of a set of balls on a simple cubic lattice gives an upper bound for the ground state energy that is sufficient for these purposes. In the dilute limit $\rho \to 0$ these droplets should move infinitely apart. Each one of the droplets should therefore be asymptotically equal to an energy-per-volume minimizer of the full-space energy functional (1.3). This is why the energy per unit volume should be given to leading order by $\inf_{0<|\Omega|<\infty} |\Omega|^{-1}\mathcal{E}_0(\Omega) = (A^*)^{-1}E_0(A^*)$.

It is a well-known open problem to prove the periodicity of minimizers in this and other, multi-dimensional minimization problems (crystallization conjecture). The strongest result about local order for the liquid drop model (in any dimension $d \in \mathbb{N}$) is shown in a work by Alberti, Choksi and Otto [1].

Remarkably, in the physics literature [43, 28] it is proposed that there are phase transitions at $0 < \rho_{c1} < \rho_{c2} < 1/2 < \rho_{c3} = 1 - \rho_{c2} < \rho_{c4} = 1 - \rho_{c1} < 1$, where the

[1]The following part of this section is similar to what has been published in [13] as joined work with Rupert Frank and Tobias König.

dimensionality of the periodicity changes. For $0 < \rho < \rho_{c1}$, minimizers are expected to be sphere shaped and arranged in a three dimensional lattice, for $\rho_{c1} < \rho < \rho_{c2}$, minimizers are expected to be cylinder shaped and arranged in a two-periodic lattice and for $\rho_{c2} < \rho < \rho_{c3}$ minimizers are expected to be slab shaped with respect to a one-dimensional lattice. For $\rho > 1/2$ the situation reverses (since $\rho \mapsto 1-\rho$ corresponds to $\Omega \mapsto \mathbb{R}^3\backslash\Omega$) and one expects a transition to cylindrical holes and then to spherical holes. Numerically, one has $\rho_{c1} \approx 0.20$ and $\rho_{c2} \approx 0.35$ [41]. In a recent result [24] the optimality of slab-like structures was rigorously established in a multi-dimensional lattice model which, similarly to the present model, contains an attractive short range term competing with a repulsive long-range term, see also [12, 26].

Theorem 2.1 improves a result of Knüpfer, Muratov and Novaga [32]. They prove a similar asymptotic equality in the ultra-dilute limit $\rho \sim L^{-2}$, where the background density vanishes in the limit $L \to \infty$. In contrast, here one can perform first the limit $L \to \infty$ and then $\rho \to 0$. In the regime $\rho \sim L^{-2}$ it does not play a role yet that the Coulomb potential is non-integrable at infinity. Controlling this phenomenon is, in fact, one of the accomplishments in this work. However, [32] also contains results about Gamma convergence and about the droplet structure of minimizers.

The even more dilute situation where $\rho \sim L^{-3}$ was considered by Choksi and Peletier [9]. Then, the leading order $E(A^*)/A^*$ in (2.3) and (2.4) should be replaced by $E(\rho L^3)/(\rho L^3)$. In this situation the upper bound (2.3) in this thesis is not applicable (at least not if ρL^3 is too small) and the lower bound (2.4) in this thesis is not tight. However, a simple variation of the arguments in this thesis would also cover this regime. Note that [9] also establishes a lower order correction to the energy and contains results about Gamma convergence.[2]

1.3 The two dimensional Liquid Drop Model

As it has been mentioned it is conjectured in the physics literature [43, 28] that there are phase transitions in nuclear matter for certain values of $\rho \in (0,1)$ where the dimensionality of the periodicity of a minimizer changes. For $\rho \in (0, \rho_{c_1})$ it is assumed that a minimizer consists of nearly spherical droplets. For $\rho \in (\rho_{c_1}, \rho_{c_2})$ it is conjectured that a minimizer consists of a parallel structure of cylinders. This phase can mathematically be described by the two dimensional liquid drop model.

In two dimensions the Newtonian potential is minus the logarithm. Therefore, the energy of the liquid drop model in $Q_L = (-L/2, L/2)^2$ is

$$\mathcal{E}_{\rho,L}(\Omega_{\rho,L}) = \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L}\int_{Q_L} (1_{\Omega_{\rho,L}}(x) - \rho) \ln \frac{1}{|x-y|} (1_{\Omega_{\rho,L}}(y) - \rho)\, \mathrm{d}x\, \mathrm{d}y\,, \tag{1.8}$$

for $\Omega_{\rho,L} \subset Q_L$ with $|\Omega_{\rho,L}| = \rho L^2$. Consider the corresponding ground state energy

$$E_{\rho,L} = \inf\Big\{\mathcal{E}_{\rho,L}(\Omega) : \Omega \subset Q_L, |\Omega| = \rho L^2\Big\}.$$

[2]End of the part of this section that is similar to what has been published.

Similar to what has been done in three dimensions the following theorem on the thermodynamic limit of the ground state energy for small $\rho > 0$ is derived in dimension two. As before this asymptotics of the thermodynamic limit also holds for Dirichlet, periodic and Neumann boundary conditions by Theorem 3.22. The energy of these boundary conditions is defined in Section 1.4.

Theorem 1.3. *Let* $\# \in \{\mathrm{Dir}, \infty, \mathrm{Per}, \mathrm{Neu}\}$*. Then, for* $\rho \in (0, \frac{1}{C})$*, the thermodynamic limit of the ground state energy for* $d = 2$ *is given by*

$$\lim_{L\to\infty} \frac{1}{L^2} E^{\#}_{\rho,L} = 3\left(\frac{\pi}{4}\ln\frac{1}{\rho}\right)^{1/3} \rho + \mathcal{O}\left(\frac{\rho}{(\ln\frac{1}{\rho})^{2/3}}\right) \quad \text{as } \rho \to 0. \tag{1.9}$$

In particular, it is equal for these boundary conditions.

Remark 1.4. This expansion of the thermodynamic limit holds for any boundary condition with a potential $v_{\rho,L}$ of the energy minimizer $\Omega_{\rho,L}$ that fulfills $\int_{\partial Q_L} v_{\rho,L} \nu \cdot \boldsymbol{\nabla} v_{\rho,L}\, \mathrm{d}x' \le 0$ for all $L \ge C$ and $\rho \in (0, \frac{1}{C})$.

In the literature sometimes a screened version of this energy is considered with an interaction that tends to zero exponentially at infinity. This avoids the difficulties that arise since the Coulomb potential is not integrable at infinity. If one considers the unscreened version $\mathcal{E}_{\rho,L}$ these difficulties can be solved by placing disks on a lattice for the upper bound such that there is local charge neutrality and such that the dipole and the quadrupole moment of each droplet with the background of one lattice cell vanish. Then, the remaining interaction at large distances $r > 0$ is of order $\frac{1}{r^3}$ which is integrable at infinity in two dimensions. This is just the method that has been used in this thesis for the three dimensional problem.

In [7] Chen and Oshita solve this issue for the upper bound by using an explicit formula for the Green function for points on a lattice on the whole of $\mathbb{R}^2$. To get an idea of how a minimizer of $\mathcal{E}_{\rho,L}$ might look like they calculate the energy of several states and compare the results. They show that a state consisting of an arrangement of discs on a hexagonal lattice has the lowest energy among several other lattice arrangements. Indeed, they calculate the energy of discs with equal radius arranged on a lattice $\alpha\mathbb{Z} + \beta\mathbb{Z}$ where $\alpha, \beta \in \mathbb{C}\backslash\{0\}$ and $\mathrm{Im}(\beta/\alpha) > 0$. Here, $\mathbb{R}^2$ is identified with $\mathbb{C}$ which simplifies calculations a lot. The lattice with hexagonal unit cell for which they got the lowest energy corresponds to $\alpha = e^{-i\pi/6}$, $\beta = e^{i\pi/6}$. They do not prove a lower bound on the ground state energy and it does not currently seem to be realistic to prove a lower bound that is equal to the upper bound of a lattice arrangement in the thermodynamic limit since this would require proving the periodicity of minimizers. As Alberti-Choksi-Otto point out, this currently is a formidable task [1].

In this thesis, a lower bound is proven that is equal to the leading order of the upper bound in (3.5) in the dilute limit $\rho \to 0$. It might be possible to even prove a lower bound that is equal to the second order, as well. Since the upper bound is stated in terms of the jellium energy a corresponding lower bound does not need to make any assumption about whether the droplets are arranged in terms of a lattice or not. This will be discussed later in greater detail.

Goldman, Muratov and Serfaty actually derive the second order asymptotics of the ground state energy for an interaction which tends to zero at infinity exponentially fast [25]. They consider the ultra-dilute limit where $\rho \propto L^{-2}(\ln \frac{1}{L})^{1/3}$ converges to zero as L tends to infinity. This is a remarkable result and their method of solving this problem has been helpful for this work as well. To prove the lower bound they show that each connected component either converges to a ball of a certain radius or becomes very small fast in the limit $\rho \to 0$.

The conjectured second order asymptotics Considering the unscreened version of the energy without coupling the limits $L \to \infty$ and $\rho \to 0$, one can conjecture that the second order of the energy for small $\rho > 0$ is

$$\left(\frac{\pi}{4}\right)^{1/3}\left(\ln \pi + \frac{1}{2} + 4e_{\text{Jellium}}\right)\frac{\rho L^2}{(\ln \frac{1}{\rho})^{2/3}},$$

where e_{Jellium} is the thermodynamic limit of the ground state energy of the jellium model. This is the second order of the upper bound proven in Theorem 3.1. The lower bound reproduces the order of the conjectured asymptotics but it does not have the conjectured coefficient.

The leading order in Theorem 3.1 comes from the part of the energy which can be expressed as

$$\sum_j \left(\sqrt{4\pi|\Omega_j|} + \frac{1}{2}\int_{\Omega_j}\int_{\Omega_j} \ln\frac{1}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y\right)$$

with $\Omega_{\rho,L} = \bigcup_j \Omega_j$, pairwise disjoint $\Omega_{j_1} \cap \Omega_{j_2} = \emptyset$ for $j_1 \neq j_2$, every Ω_j connected and $\operatorname{diam}(\Omega_j) \leq C(\ln \frac{1}{\rho})^{2/3}$. It actually does not depend on the shape of the Ω_j but only on the mass $|\Omega_j|$ and the perimeter $\operatorname{Per}\Omega_j$. The contribution of the shape is of subleading order.

Consequently, the next order is contained in the energy

$$\sum_j \left(\operatorname{Per}(\Omega_j) - \sqrt{4\pi|\Omega_j|}\right) + \frac{1}{2}\int_{Q_L}\int_{Q_L} (1_{\Omega_{\rho,L}}(x) - \rho)\ln\frac{1}{|x-y|}(1_{\Omega_{\rho,L}}(y) - \rho)\,\mathrm{d}x\,\mathrm{d}y$$
$$- \sum_j \frac{1}{2}\int_{\Omega_j}\int_{\Omega_j} \ln\frac{1}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y\,.$$

The first term gives control over the difference of each connected component and a ball by the quantitative isoperimetric inequality. The second term is precisely the Coulomb energy without the self-energy of the connected components.

Since the first term favors connected components to be like a ball one expects the second term to be similar to the jellium energy. The advantage of this approach is that one only has to get results about the mass and shape of the droplets and that one does not need to make any assumption about whether the droplets are arranged in terms of a lattice. The proof of the lower bound in Theorem 3.1 actually shows that most droplets of a minimizer have mass less then $C(\ln\frac{1}{\rho})^{-2/3}$ and perimeter less then $C(\ln\frac{1}{\rho})^{-1/3}$. If droplets Ω_i either have mass larger than that or a perimeter that is larger than this, then their energy is greater than $C_0(\ln\frac{1}{\rho})^{1/3}|\Omega_i|$ with $C_0 > 3(\frac{\pi}{4})^{1/3}$. So the sum of these masses $|\Omega_i|$ fullfills

$$3\Big(\frac{\pi}{4}\ln\frac{1}{\rho}\Big)^{1/3}\sum_j|\Omega_j| + C_0\Big(\ln\frac{1}{\rho}\Big)^{1/3}\sum_i|\Omega_i| \le 3\Big(\frac{\pi}{4}\ln\frac{1}{\rho}\Big)^{1/3}|\Omega_{\rho,L}| + \frac{C|\Omega_{\rho,L}|}{(\ln\frac{1}{\rho})^{2/3}}$$
$$\iff \frac{\sum_i|\Omega_i|}{|\Omega_{\rho,L}|} \le \frac{C}{\ln\frac{1}{\rho}}.$$

Here, the sum over j denotes all droplets Ω_j that have mass less then $C(\ln\frac{1}{\rho})^{-2/3}$ and perimeter less than $C(\ln\frac{1}{\rho})^{-1/3}$. Their energy is bound from below by $3(\frac{\pi}{4}\ln\frac{1}{\rho})^{1/3}|\Omega_j|$ (as the proof of the lower bound shows). One can improve on this argument similar to what Goldman, Muratov, Serfaty show in [25] and deduce that most droplet masses asymptotically converge to an optimal mass and that their shape converges to that of a ball. This is done in Chapter 3 as well.

1.4 Concerning boundary conditions

This section is similar to what has been published in [13] with Rupert Frank and Tobias König in three dimensions.

In the literature the liquid drop model energy (1.1) is often considered with different boundary conditions like Dirichlet, Neumann or periodic ones. To introduce the corresponding energies, the liquid drop model energy is written in terms of the potential, first. For $\Omega_{\rho,L} \subset Q_L$ with $|\Omega_{\rho,L}| = \rho L^d$, let $v^\infty_{\rho,L}$ be the solution of the whole space problem

$$\begin{cases} -\Delta v^\infty_{\rho,L} = c_d(1_{\Omega_{\rho,L}} - \rho 1_{Q_L}) & \text{in } \mathbb{R}^d, \\ v^\infty_{\rho,L} \in H^1(\mathbb{R}^d), \end{cases} \tag{1.10}$$

where $c_d := (d-2)|\mathbb{S}^{d-1}|$ for $d \ge 3$, $c_2 := 2\pi$ and with $G(x) = \frac{1}{|x|^{d-2}}$ in dimension $d \ge 3$ and $G(x) = \ln\frac{1}{|x|}$ in dimension $d = 2$. Integrating by parts gives

$$\begin{aligned}\mathcal{E}_{\rho,L}(\Omega_{\rho,L}) &= \operatorname{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}(1_{\Omega_{\rho,L}}(x) - \rho 1_{Q_L}(x))G(x-y)(1_{\Omega_{\rho,L}}(y) - \rho 1_{Q_L}(y))\,\mathrm{d}x\,\mathrm{d}y \\ &= \operatorname{Per}(\Omega_{\rho,L}) + \frac{1}{2c_d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}(-\Delta v^\infty_{\rho,L})v^\infty_{\rho,L}\,\mathrm{d}x \\ &= \operatorname{Per}(\Omega_{\rho,L}) + \frac{1}{2c_d}\int_{\mathbb{R}^d}\left|\nabla v^\infty_{\rho,L}\right|^2\mathrm{d}x\,.\end{aligned}$$

To define the liquid drop model energy for different boundary conditions, suppose $v^{\mathrm{Dir}}_{\rho,L}, v^{\mathrm{Neu}}_{\rho,L} \in H^1(Q_L)$ and $v^{\mathrm{Per}}_{\rho,L} \in H^1(\mathbb{R}^d)$. For $\# \in \{\mathrm{Dir},\mathrm{Per},\mathrm{Neu}\}$ let $v^\#_{\rho,L}$ be the solution of

$$-\Delta v^\#_{\rho,L} = c_d(1_{\Omega_{\rho,L}} - \rho) \qquad \text{in } Q_L \tag{1.11}$$

with the corresponding boundary condition $v_{\rho,L}^{\mathrm{Dir}}(x) = 0$ and $\nu \cdot \boldsymbol{\nabla} v_{\rho,L}^{\mathrm{Neu}}(x) = 0$ for $x \in \partial Q_L$ and $v_{\rho,L}^{\mathrm{Per}}(x + rL) = v_{\rho,L}^{\mathrm{Per}}(x)$ for all $r \in \mathbb{Z}^d$ and $x \in \mathbb{R}^d$. Then, define the energy functional

$$\mathcal{E}_{\rho,L}^{\#}(\Omega_{\rho,L}) := \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2c_d} \int_{Q_L} \left| \boldsymbol{\nabla} v_{\rho,L}^{\#} \right|^2 \mathrm{d}x \,, \tag{1.12}$$

and denote the corresponding ground state energy by

$$E_{\rho,L}^{\#} := \inf\{\mathcal{E}_{\rho,L}^{\#}(\Omega) : \Omega \subset Q_L, |\Omega| = \rho L^d\}. \tag{1.13}$$

for $\# \in \{\mathrm{Dir}, \mathrm{Per}, \mathrm{Neu}\}$. Note that sometimes for the whole space energy the analogous notation is used $\mathcal{E}_{\rho,L}^{\infty} := \mathcal{E}_{\rho,L}$ and $E_{\rho,L}^{\infty} := E_{\rho,L}$.

The energy of the Dirichlet problem is less than the one of the problem with whole space or periodic boundary conditions which again are less than the energy of the Neumann problem. Indeed, let $\# \in \{\infty, \mathrm{Per}, \mathrm{Neu}\}$, then

$$\begin{aligned}
\mathcal{E}_{\rho,L}^{\#}(\Omega_{\rho,L}) &\geq \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2c_d} \int_{Q_L} \left| \boldsymbol{\nabla} v_{\rho,L}^{\#} \right|^2 \mathrm{d}x \\
&= \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2c_d} \int_{Q_L} \left| \boldsymbol{\nabla} v_{\rho,L}^{\mathrm{Dir}} + \boldsymbol{\nabla} v_{\rho,L}^{\#} - \boldsymbol{\nabla} v_{\rho,L}^{\mathrm{Dir}} \right|^2 \mathrm{d}x \\
&\geq \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2c_d} \int_{Q_L} \left| \boldsymbol{\nabla} v_{\rho,L}^{\mathrm{Dir}} \right|^2 \mathrm{d}x + \frac{1}{c_d} \int_{Q_L} \boldsymbol{\nabla} v_{\rho,L}^{\mathrm{Dir}} \cdot \left(\boldsymbol{\nabla} v_{\rho,L}^{\#} - \boldsymbol{\nabla} v_{\rho,L}^{\mathrm{Dir}} \right) \mathrm{d}x \\
&= \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2c_d} \int_{Q_L} \left| \boldsymbol{\nabla} v_{\rho,L}^{\mathrm{Dir}} \right|^2 \mathrm{d}x + \frac{1}{c_d} \int_{Q_L} v_{\rho,L}^{\mathrm{Dir}} \left(-\Delta v_{\rho,L}^{\#} + \Delta v_{\rho,L}^{\mathrm{Dir}} \right) \mathrm{d}x \\
&\quad + \frac{1}{c_d} \int_{\partial Q_L} v_{\rho,L}^{\mathrm{Dir}} \nu \cdot \left(\boldsymbol{\nabla} v_{\rho,L}^{\#} - \boldsymbol{\nabla} v_{\rho,L}^{\mathrm{Dir}} \right) \mathrm{d}x' \\
&= \mathcal{E}_{\rho,L}^{\mathrm{Dir}}(\Omega_{\rho,L}),
\end{aligned}$$

since $-\Delta v_{\rho,L}^{\#} = 1_{\Omega_{\rho,L}} - \rho = -\Delta v_{\rho,L}^{\mathrm{Dir}}$ in Q_L and $v_{\rho,L}^{\mathrm{Dir}}(x) = 0$ for $x \in \partial Q_L$. It is clear that the specific form of boundary condition for $v_{\rho,L}^{\#}$ is not needed to bound the energy from below by the Dirichlet energy.

Furthermore,

$$\begin{aligned}
\int_{\mathbb{R}^d \backslash Q_L} \left| \boldsymbol{\nabla} v_{\rho,L}^{\infty} \right|^2 \mathrm{d}x &= \int_{\mathbb{R}^d \backslash Q_L} v_{\rho,L}^{\infty} \left(-\Delta v_{\rho,L}^{\infty} \right) \mathrm{d}x - \int_{\partial Q_L} v_{\rho,L}^{\infty} \nu \cdot \boldsymbol{\nabla} v_{\rho,L}^{\infty} \, \mathrm{d}x' \\
&= -\int_{\partial Q_L} v_{\rho,L}^{\infty} \nu \cdot \boldsymbol{\nabla} v_{\rho,L}^{\infty} \, \mathrm{d}x' \,,
\end{aligned}$$

because $-\Delta v_{\rho,L}^{\infty} = 0$ in $\mathbb{R}^d \backslash Q_L$ and for ν being the outer normal vector of ∂Q_L.

Therefore, integrating by parts gives

$$\begin{aligned}
\mathcal{E}_{\rho,L}^{\mathrm{Neu}}(\Omega_{\rho,L}) &= \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2c_d} \int_{Q_L} \left| \boldsymbol{\nabla} v_{\rho,L}^{\infty} + \boldsymbol{\nabla} v_{\rho,L}^{\mathrm{Neu}} - \boldsymbol{\nabla} v_{\rho,L}^{\infty} \right|^2 \mathrm{d}x \\
&\geq \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2c_d} \int_{Q_L} \left| \boldsymbol{\nabla} v_{\rho,L}^{\infty} \right|^2 \mathrm{d}x + \frac{1}{c_d} \int_{Q_L} \boldsymbol{\nabla} v_{\rho,L}^{\infty} \cdot \left(\boldsymbol{\nabla} v_{\rho,L}^{\mathrm{Neu}} - \boldsymbol{\nabla} v_{\rho,L}^{\infty} \right) \mathrm{d}x \\
&= \mathcal{E}_{\rho,L}^{\infty}(\Omega_{\rho,L}) - \frac{1}{2c_d} \int_{\mathbb{R}^d \backslash Q_L} \left| \boldsymbol{\nabla} v_{\rho,L}^{\infty} \right|^2 \mathrm{d}x + \frac{1}{c_d} \int_{\partial Q_L} v_{\rho,L}^{\infty} \nu \cdot \left(\boldsymbol{\nabla} v_{\rho,L}^{\mathrm{Neu}} - \boldsymbol{\nabla} v_{\rho,L}^{\infty} \right) \mathrm{d}x' \\
&\geq \mathcal{E}_{\rho,L}^{\infty}(\Omega_{\rho,L})
\end{aligned}$$

since $-\Delta v^{\mathrm{Neu}}_{\rho,L} = 1_{\Omega_{\rho,L}} - \rho = -\Delta v^{\infty}_{\rho,L}$ in Q_L and $\nu \cdot \nabla v^{\mathrm{Neu}}_{\rho,L} = 0$ on ∂Q_L.

A similar calculation shows $\mathcal{E}^{\mathrm{Neu}}_{\rho,L}(\Omega_{\rho,L}) \geq \mathcal{E}^{\mathrm{Per}}_{\rho,L}(\Omega_{\rho,L})$ since $\int_{\partial Q_L} v^{\mathrm{Per}}_{\rho,L} \nu \cdot \nabla v^{\mathrm{Per}}_{\rho,L} \, \mathrm{d}x' = 0$. Actually, the energy of any boundary condition can be bounded from above by the Neumann energy if the potential $v_{\rho,L}$ of the minimizer $\Omega_{\rho,L}$ fulfills the assumption $\int_{\partial Q_L} v_{\rho,L} \, \nu \cdot \nabla v_{\rho,L} \, \mathrm{d}x' \leq 0$ for all $L > C$ and $\rho \in (0, \frac{1}{2}]$.

Thus, for $\# \in \{\infty, \mathrm{Per}\}$ and for any $\Omega_{\rho,L} \subset Q_L$ with $|\Omega_{\rho,L}| = \rho L^d$ one has

$$\mathcal{E}^{\mathrm{Dir}}_{\rho,L}(\Omega_{\rho,L}) \leq \mathcal{E}^{\#}_{\rho,L}(\Omega_{\rho,L}) \leq \mathcal{E}^{\mathrm{Neu}}_{\rho,L}(\Omega_{\rho,L}). \tag{1.14}$$

Note that this inequality does not require to take the thermodynamic limit.

In Chapter 3 it is shown that the thermodynamic limit exists and is equal for Dirichlet, whole space, periodic and Neumann boundary conditions. In particular this implies that the results on the ground state energy for small $\rho > 0$ in dimension $d \in \{2, 3\}$ derived in Chapters 2 and 3 are also valid for Dirichlet, periodic and Neumann boundary conditions in the thermodynamic limit.

1.5 Uniform Distribution of Energy and Existence of the Thermodynamic Limit

Having the correct leading order constant in the dilute limit $\rho \to 0$ in two and three dimensions, one might ask whether the energy of the liquid drop model is uniformly distributed throughout Q_L and what the minimal length scale is that one can prove this uniform distribution of energy for.

Alberti, Choksi and Otto prove uniform distribution of energy in d dimensions with $d \in \mathbb{N}$ down to the constant scale (with respect to L) in [1]. However, it is not clear how the constant depends on the charge density $\rho > 0$.

The expected length scale for the minimal distance of two connected components of a minimizer is $l \propto (\ln \frac{1}{\rho})^{-1/3} \rho^{-1/2}$ in two dimensions and $l \propto \rho^{-1/3}$ in three dimensions. So the result one would hope to prove is getting a minimal length scale of uniform distribution of energy $C c_{d,\rho}^{-1} \rho^{-1/d}$ for some large $C > 0$. Here $c_{2,\rho} := (\ln \frac{1}{\rho})^{1/3}$ and $c_{d,\rho} := 1$ for $d \geq 3$.

In this thesis uniform distribution of energy (with correct leading order coefficient) is proven down to scale $C c_{d,\rho}^{1/2} \rho^{-1/2}$. So, in two dimensions the result is only by a factor of $(\ln \frac{1}{\rho})^{1/2}$ above the conjectured minimal length scale. In three dimensions it is a factor of $\rho^{-1/6}$.

If $d = 2$ and if one does not want an error which is greater than the error in Theorem 3.1, that is $C\rho(\ln \frac{1}{\rho})^{-2/3}$, the result requires a length scale greater than $C(\ln \frac{1}{\rho})^{5/3} \rho^{-1/2}$.

The proof presented in this thesis is similar to the proof of Theorem 4 in [2]. There, Armstrong and Serfaty prove uniform distribution of energy for the jellium model. The techniques they use can be simplified in case of the liquid drop model.

Before sketching the idea of this proof, the following reformulation of the liquid drop model energy is needed which Alberti, Choksi and Otto consider in [1]. Instead of writing the Coulomb energy in terms of the potential one just writes it in terms of the electric field (which is denoted by **b**). This is essential for the proof of uniform distribution of energy since it allows for cutting and pasting arguments.

Throughout this section it is assumed $d \in \mathbb{N}$ with $d \geq 2$.

The energy in terms of the electric field Consider $Q \subseteq \mathbb{R}^d$, a set $\Omega \subset \mathbb{R}^d$ representing the nuclear matter and the corresponding electric field $\mathbf{b} \in L^2(Q, \mathbb{R}^d)$. As in [1], define

$$\mathcal{E}(\Omega, \mathbf{b}, Q) := \mathrm{Per}(\Omega \cap Q) + \frac{1}{2} \int_Q |\mathbf{b}|^2 \, \mathrm{d}x \,. \tag{1.15}$$

Often one sets $Q = Q_L = (-L/2, L/2)^d$, so if $\Omega \subset Q_L$, abbreviate $\mathcal{E}(\Omega, \mathbf{b}) := \mathcal{E}(\Omega, \mathbf{b}, Q_L)$.

Uniform distribution of energy will be proven in case of Neumann boundary conditions

$$\mathcal{A}_{\mathrm{Neu}}(\rho, Q) := \Big\{(\rho, Q) \mid \Omega \subset Q \text{ and } \mathbf{b} \in L^2(Q, \mathbb{R}^d) \text{ with } |\Omega| = \rho|Q| \text{ such that } \\ \boldsymbol{\nabla} \mathbf{b} = 1_\Omega - \rho \text{ in } Q \text{ and } \mathbf{b} \cdot \nu = 0 \text{ on } \partial Q\Big\}.$$

Furthermore, define the whole space boundary condition and the Dirichlet boundary condition

$$\mathcal{A}_{\infty}(\rho, Q) := \Big\{(\rho, Q) \mid \Omega \subset Q \text{ and } \mathbf{b} \in L^2(\mathbb{R}^d, \mathbb{R}^d) \text{ with } |\Omega| = \rho|Q| \text{ such that } \\ \boldsymbol{\nabla} \mathbf{b} = 1_\Omega - \rho 1_Q \text{ in } \mathbb{R}^d\Big\},$$

$$\mathcal{A}_{\mathrm{Dir}}(\rho, Q) := \Big\{(\rho, Q) \mid \Omega \subset Q \text{ and } \mathbf{b} \in L^2(Q, \mathbb{R}^d) \text{ with } |\Omega| = \rho|Q| \text{ such that } \\ \boldsymbol{\nabla} \mathbf{b} = 1_\Omega - \rho \text{ in } Q\Big\}.$$

Denote the corresponding ground state energies by

$$E_{\#}(\rho, Q) := \inf \Big\{\mathcal{E}(\Omega, \mathbf{b}, Q) : (\Omega, \mathbf{b}) \in \mathcal{A}_{\#}(\rho, Q)\Big\},$$

with $\# \in \{\mathrm{Neu}, \mathrm{Dir}\}$ and $E_\infty(\rho, Q) := \inf\{\mathcal{E}(\Omega, \mathbf{b}, \mathbb{R}^d) : (\Omega, \mathbf{b}) \in \mathcal{A}_\infty(\rho, Q_L)\}$.

Clearly, one has $E_{\mathrm{Dir}}(\rho, Q) \leq E_\infty(\rho, Q) \leq E_{\mathrm{Neu}}(\rho, Q)$ because one can identify $(\Omega, \mathbf{b}) \in \mathcal{A}_{\mathrm{Neu}}(\rho, Q)$ with $\mathbf{b} \in L^2(\mathbb{R}^d)$ extended by 0 in $\mathbb{R}^d \backslash Q$. Then, $(\Omega, \mathbf{b}) \in \mathcal{A}_\infty(\rho, Q)$. And one can simply restrict $(\Omega, \mathbf{b}) \in \mathcal{A}_\infty(\rho, Q)$ to $(\Omega, \mathbf{b}|_Q) \in \mathcal{A}_{\mathrm{Dir}}(\rho, Q)$.

Making use of the monotonicity of the Neumann and Dirichlet energies as in [1], later on in Chapter 3 it is proven that the thermodynamic limits $e_{\#}(\theta) := \lim_{L\to\infty} \frac{1}{L^d} E_{\#}(\rho, Q_L)$ exist for $\# \in \{\mathrm{Neu}, \mathrm{Dir}\}$ and that they are equal. This also implies the existence and equality of the thermodynamic limit of the ground state energy with whole space or periodic boundary conditions.

The main result of this chapter is the following theorem. The error is better if small length scales R are considered. With a similar method a result for large length scales can be proven such that the error term is of order $\mathcal{O}(R^{d-1})$.

Theorem 1.5 (Uniform distribution of energy)**.** *Let $(\Omega_{\rho,L}, \mathbf{b}_{\rho,L})$ be a minimizer of $\mathcal{E}(\cdot,\cdot,Q_L)$ over $\mathcal{A}_{\mathrm{Neu}}(\rho, Q_L)$. Suppose $\rho \in (0, \frac{1}{2}]$ and $L \geq R \geq C\delta^{-(d+1)/2} c_{d,\rho}^{1/2} \rho^{-1/2}$. For $a \in Q_L$ such that $Q_R(a) \subset Q_L$ one has*

$$\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a)) = E_{\mathrm{Neu}}(\rho, Q_R(a)) + \mathcal{O}(\delta c_{d,\rho} \rho R^d), \tag{1.16}$$

if the boundary can be estimated $\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_R(a) \backslash \partial Q_L) \leq C\delta c_{d,\rho} \rho R^d$.

Remark 1.6. This condition on the boundary is always fulfilled if R is sufficiently large. If smaller length scales are considered, one can make use of neutrality to find a good boundary by averaging.

Note that this result is particularly interesting in the dilute limit which has been considered so far in this thesis. Alberti, Choksi and Otto prove a remarkable result on the uniform distribution of energy [1] but the dependence of the constant on the density $\rho > 0$ is not clear. If one tracks this dependence throughout their proof it becomes clear that their constant actually gets worse for small $\rho > 0$, i.e. it tends to infinity like $\frac{1}{\rho^n}$ for some $n > 0$. The error in this estimate actually gets better for $\rho \to 0$.

Equivalence of the electric field and the Coulomb potential energies In the introduction of [1] it is shown that the ground state energy is the same whether one minimizes over electric fields or just writes the energy in terms of the Coulomb potential. As it helps understanding this formulation this short proof is given below.

Let $\Omega_{\rho,L} \subset Q_L$ with $|\Omega_{\rho,L}| = \rho L^d$ and let $v_{\rho,L} \in H^2(Q_L)$ be such that $-\Delta v_{\rho,L} = 1_{\Omega_{\rho,L}} - \rho$ in Q_L. Later it will be specified which boundary condition $v_{\rho,L}$ should fulfill. For any $\mathbf{b}_{\rho,L} \in L^2(Q_L)$ with $\boldsymbol{\nabla} \mathbf{b}_{\rho,L} = 1_{\Omega_{\rho,L}} - \rho$ in Q_L in the sense of distributions, one has

$$\begin{aligned}
&\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}) = \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L} |\mathbf{b}_{\rho,L}|^2 \,\mathrm{d}x \\
&= \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L} |-\boldsymbol{\nabla} v_{\rho,L} + \mathbf{b}_{\rho,L} + \boldsymbol{\nabla} v_{\rho,L}|^2 \,\mathrm{d}x \\
&= \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L} \Big(|\boldsymbol{\nabla} v_{\rho,L}|^2 - 2\boldsymbol{\nabla} v_{\rho,L} \cdot (\mathbf{b}_{\rho,L} + \boldsymbol{\nabla} v_{\rho,L}) + |\mathbf{b}_{\rho,L} + \boldsymbol{\nabla} v_{\rho,L}|^2 \Big) \,\mathrm{d}x \\
&\geq \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L} \Big(|\boldsymbol{\nabla} v_{\rho,L}|^2 + 2v_{\rho,L}(\nabla \mathbf{b}_{\rho,L} + \Delta v_{\rho,L}) \Big) \,\mathrm{d}x - \int_{\partial Q_L} v_{\rho,L}(\mathbf{b}_{\rho,L} + \boldsymbol{\nabla} v_{\rho,L}) \cdot \nu \,\mathrm{d}x' \\
&= \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L} |\boldsymbol{\nabla} v_{\rho,L}|^2 \,\mathrm{d}x - \int_{\partial Q_L} v_{\rho,L}(\mathbf{b}_{\rho,L} + \boldsymbol{\nabla} v_{\rho,L}) \cdot \nu \,\mathrm{d}x',
\end{aligned}$$

since $\nabla \mathbf{b}_{\rho,L} = 1_{\Omega_{\rho,L}} - \rho = -\Delta v_{\rho,L}$ in Q_L. If both $\mathbf{b}_{\rho,L}$ and $v_{\rho,L}$ fulfill the Neumann boundary condition, that is if $\mathbf{b}_{\rho,L} \cdot \nu = 0$ on ∂Q_L and $\nu \cdot \boldsymbol{\nabla} v_{\rho,L} = 0$ on ∂Q_L, then the boundary integral is zero. If $v_{\rho,L}$ fulfills Dirichlet boundary condition, that is if $v_{\rho,L} = 0$ on ∂Q_L, then no assumption about the boundary of $\mathbf{b}_{\rho,L}$ is needed. The boundary integral vanishes, anyway.

A similar calculation also holds for whole space boundary conditions. The integral over Q_L is simply replaced by an integral over $\mathbb{R}^d$ and thus, there is no boundary term.

If $v^{\#}_{\rho,L}$ fulfills a given boundary condition $\# \in \{\text{Dir}, \text{Neu}\}$ for some $\Omega_{\rho,L} \subset Q_L$ with $|\Omega_{\rho,L}| = \rho L^d$, clearly, one has $\nabla v^{\#}_{\rho,L} \in \mathcal{A}_{\#}(\rho, Q_L)$ and therefore,

$$\mathcal{E}(\Omega_{\rho,L}, \nabla v^{\#}_{\rho,L}, Q_L) = \inf\{\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_L) : (\Omega_{\rho,L}, \mathbf{b}_{\rho,L}) \in \mathcal{A}_{\#}(\rho, Q_L)\}. \tag{1.17}$$

Similarly, $\mathcal{E}(\Omega_{\rho,L}, \nabla v^{\infty}_{\rho,L}, \mathbb{R}^d) = \inf\{\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, \mathbb{R}^d) : (\Omega_{\rho,L}, \mathbf{b}_{\rho,L}) \in \mathcal{A}_{\infty}(\rho, Q_L)\}$. This justifies the previous definition of $\mathcal{A}_{\text{Dir}}(\rho, Q_L)$ which might not have been obvious.

Note that the ground state energy of the formulation in terms of electric field $E_{\#}(\rho, Q_L)$ has to be rescaled compared to the definition of the ground state energy in terms of the Coulomb potential $E^{\#}_{\rho,L}$. Indeed, for whole space boundary conditions one has $E_{\infty}(\rho, Q_L) = c_d^{\frac{d-1}{3}} E^{\infty}_{\rho, L c_d^{-1/3}}$ with $c_2 = 2\pi$ and $c_d = (d-2)|\mathbb{S}^{d-1}|$ (not to be confused with $c_{d,\rho}$).

Uniform distribution of energy To sketch the idea of the proof that is similar to the proof of Theorem 4 by Armstrong and Serfaty in [2], let $(\Omega, \mathbf{b})$ be a minimizer of $\mathcal{E}(\cdot, \cdot, Q_L)$ over $\mathcal{A}_{\text{Neu}}(\rho, Q_L)$. One would like to prove the upper bound for $R \le L$ and $a \in Q_L$ such that $Q_R(a) \subseteq Q_L$

$$\mathcal{E}(\Omega, \mathbf{b}, Q_R(a)) \le E_{\text{Neu}}(\rho, Q_R(a)) + C c^n_{d,\rho} \rho^{1-\epsilon} R^{d-2\epsilon},$$

without specifying $n \in \mathbb{R}$ and $\epsilon > 0$ at the moment. As previously defined $c_{2,\rho} := (\ln \frac{1}{\rho})^{1/3}$ and $c_{d,\rho} := 1$ for $d \ge 3$.

The basic idea of proving this is a cutting and pasting argument. Let $(\Omega_0, \mathbf{b}_0)$ be a minimizer of $\mathcal{E}(\cdot, \cdot, Q_R(a))$ over $\mathcal{A}_{\text{Neu}}(\rho, Q_R(a))$. Define $\tilde{\Omega} := \Omega \backslash Q_R(a) \cup \Omega_0$ and

$$\tilde{\mathbf{b}}(x) := \begin{cases} \mathbf{b}(x) & \text{in } Q_L \backslash Q_R(a), \\ \mathbf{b_0}(x) & \text{in } Q_R(a). \end{cases}$$

One would then like to do the simple calculation

$$\begin{aligned} &\mathcal{E}(\Omega, \mathbf{b}, Q_R(a)) + \mathcal{E}(\Omega, \mathbf{b}, Q_L \backslash Q_R(a)) = \mathcal{E}(\Omega, \mathbf{b}, Q_L) \\ &= E_{\text{Neu}}(\rho, Q_L) \le \mathcal{E}(\tilde{\Omega}, \tilde{\mathbf{b}}, Q_L) = \mathcal{E}(\Omega_0, \mathbf{b}_0, Q_R(a)) + \mathcal{E}(\Omega, \mathbf{b}, Q_L \backslash Q_R(a)) \\ &= E_{\text{Neu}}(\rho, Q_R(a)) + \mathcal{E}(\Omega, \mathbf{b}, Q_L \backslash Q_R(a)). \end{aligned}$$

This would imply the upper bound. Actually, the perimeter term is not quite additive. One gets an additional surface term in $\partial Q_R(a)$. But this is not the main difficulty. The calculation above is wrong because one does not have $(\tilde{\Omega}, \tilde{\mathbf{b}}) \in \mathcal{A}_{\text{Neu}}(\rho, Q_L)$ in general. It does not necessarily fulfill the charge neutrality condition $|\tilde{\Omega}| = \rho L^2$. One has $|\Omega_0| = \rho R^2$, but there is no reason to assume $|\Omega \backslash Q_R(a)| = \rho(L^2 - R^2)$.

The idea taken from the work of Armstrong and Serfaty [2] is to modify $\tilde{\Omega}$ in $Q_L \backslash Q_R(a)$ such that one has neutrality $|\tilde{\Omega} \backslash Q_R(a)| = \rho^2(L^2 - R^2)$ and such that $\tilde{\mathbf{b}} \cdot \nu$ is continuous on $\partial Q_R(a)$ where ν is the outer normal vector of $\partial Q_R(a)$. For this construction to work one chooses a better boundary $Q_T(a)$ with $T \in [R + \tilde{l}, R + 2\tilde{l}]$ such that one is closer to neutrality $|\Omega \cup Q_T(a)| \approx \rho T^d$.

To make this connection between the boundary and charge neutrality more precise remember that for $(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}) \in \mathcal{A}_{\text{Neu}}(\rho, Q_L)$ one has $\nabla \mathbf{b}_{\rho,L} = 1_{\Omega_{\rho,L}} - \rho$ in Q_L. Therefore, the Gauss-Green theorem implies

$$\begin{aligned}\left||\Omega_{\rho,L} \cap Q_R(a)| - \rho R^2\right| &= \left|\int_{Q_R(a)} (1_{\Omega_{\rho,L}}(x) - \rho)\,\mathrm{d}x\right| \\ &= \left|\int_{Q_R(a)} \nabla \mathbf{b}_{\rho,L}\,\mathrm{d}x\right| = \left|\int_{\partial Q_R(a)} \mathbf{b}_{\rho,L} \cdot \nu\,\mathrm{d}x'\right| \\ &\le C\sqrt{R^{d-1}}\sqrt{\int_{\partial Q_R(a)} |\mathbf{b}_{\rho,L}|^2\,\mathrm{d}x'}.\end{aligned}$$

By averaging a $T \in [R + \tilde{l}, R + 2\tilde{l}]$ is found such that $\int_{\partial Q_T(a)} |\mathbf{b}_{\rho,L}|^2\,\mathrm{d}x'$ is not too large. Then, one knows that $||\Omega_{\rho,L} \cap Q_T(a)| - \rho T^2|$ is not too large, either. So one has found a cube that is not too far away from neutrality.

As in [2], the proof is based on a bootstrap of scales starting with $L_0 := L$ and then arguing that uniform distribution of energy holds for all $R \ge L_0/2$. Iterating this argument gives the desired result.

Large length scales A future project might be to derive a theorem that is particularly suited for large scales $R \gg \rho^{-1}$ with the method by Armstrong and Serfaty [2]. Then, factors depending on ρ are not important whereas the exponent of the error term R^{d-1} is very important. The idea of this proof would basically be the same as for the one considered in this thesis. However, the averaging argument has to be applied locally such that a piecewise affine boundary is found that fulfills local energy estimates.

The thermodynamic limit Although the Coulomb potential is not integrable on $\mathbb{R}^d$, the thermodynamic limit of the ground state energy of the liquid drop model exists. This fact can be explained by local charge neutrality (as one can explicitly see in the upper bounds of the energy in dimensions two and three). The droplets and the background of opposite charge cancel the leading orders of the Coulomb interaction. This effect is called screening. So effectively any droplet only interacts with other droplets and the background up to a range of $C(\rho)$ with interaction energy greater than a small $\epsilon(\rho) > 0$.

This is why the boundary condition should not matter in the thermodynamic limit. In Chapter 3 a theorem is derived that shows that the thermodynamic limit exists and is equal for Dirichlet, whole space and Neumann boundary conditions. Actually a whole range of boundary conditions can be considered including periodic ones. One also expects the structure of minimizers to be independent of the boundary condition in the thermodynamic limit.

1.6 Mathematical Quantum Mechanics

The second Coulomb system that is considered in this thesis is described by quantum mechanics. (For a more detailed introduction to the quantum mechanics of many particles e.g. refer to [35].)

Quantum mechanics is formulated in terms of a beautiful mathematical theory, namely functional analysis. Every observable corresponds to a self-adjoint operator on a Hilbert space $\mathcal{H}$ and the spectrum of this operator are the values one mighty possibly measure for this observable in experiments. The operator corresponding to the energy of the system is the Hamiltonian H. A physical state is a normalized vector $\psi \in \mathcal{H}$. The energy of the system in the state ψ is given by $(\psi, H\psi)$, where $(\cdot,\cdot)$ denotes the inner product on $\mathcal{H}$.

As a simple example consider just one particle in three dimensional Euclidean space $\mathcal{H} := H^2(\mathbb{R}^3)$. Then $|\psi(x)|$ is the probability density for the particle being found at $x \in \mathbb{R}^3$. The kinetic energy is described by $H = -\Delta$, so the energy of the system in ψ is $(\psi, -\Delta\psi) = \|\nabla\psi\|^2_{L^2(\mathbb{R}^3)}$.

Starting with the Hilbert space $\mathcal{H} = H^2(\mathbb{R}^3)$ of one particle and a one particle operator like the kinetic energy $H = -\Delta$, one can consider a system of N particles. The corresponding Hilbert space is $\mathcal{H}_N := H^2((\mathbb{R}^3)^N)$ and a one particle operator $H = -\Delta$ induces an operator H_N by separately applying H to every particle, that is

$$H_N := \sum_{i=1}^{N}(-\Delta_{x_i})$$

where $x = (x_1, \ldots, x_N) \in (\mathbb{R}^3)^N$.

Similarly an interaction of two particles that is described by a potential $V : \mathbb{R}^3 \to \mathbb{R}$ (for instance the Coulomb potential $V(x) = \frac{1}{|x-y|}$) induces an operator on $\mathcal{H}_N$ by letting it act on each pair of two particles separately. Thus, the total Coulomb energy of the system is described by the multiplication operator

$$\sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|}. \tag{1.18}$$

Symmetry One of the basics of quantum mechanics is that a wave function $\psi \in \mathcal{H}_N$ describing N identical particles is either antisymmetric or symmetric. Indeed, let $i, j \in \{1, \ldots, N\}, i < j$, ψ is called *antisymmetric* if and only if

$$\psi(x_1, \ldots, x_N) = (-1)^s \psi(x_1, \ldots, x_{i-1}, x_j, x_{i+1}, \ldots, x_{j-1}, x_i, x_{j+1}, \ldots, x_N), \tag{1.19}$$

for any $(x_1, \ldots, x_N) \in (\mathbb{R}^3)^N$ and for $s = 1$. If this property holds for $s = 0$, ψ is called *symmetric*.

The basic constituents of matter, protons, neutrons and electrons are particles described by an antisymmetric wave function. They are called *fermions*. Some atomic nuclei are fermions as well, some are described by a symmetric wave function. These are called *bosons*.

The direct sum of the Hilbert spaces of all possible particle numbers in case of bosons is called bosonic Fock space

$$\mathcal{F}_{\text{sym}}(\mathcal{H}) := \bigoplus_{N=0}^{\infty} \bigotimes_{\text{sym}}^{N} \mathcal{H} \tag{1.20}$$

where $\bigotimes_{\text{sym}}^{N}$ is the symmetric N-fold tensor product. A one-particle operator $H : \mathcal{H} \to \mathcal{H}$ induces an operator $Q(H)$

$$Q(H) := \sum_{N=0}^{\infty} H_N \tag{1.21}$$

on $\mathcal{F}_{\text{sym}}(\mathcal{H})$ where H_N only acts on $\bigotimes_{\text{sym}}^{N} \mathcal{H}$. $Q(H)$ is called the *second quantization* of H.

The fermionic Fock space is defined similarly with the antisymmetric tensor product of the one-particle Hilbert space $\mathcal{H}$.

In Chapter 4 of this thesis the Fock space $\mathcal{F}_{\text{sym}}(L^2(\mathbb{R}^3))$ is considered.

Let $(u_n)_{n\in\mathbb{N}}$ be an orthonormal basis of $\mathcal{H}$ (which is assumed to be separable) and let $f \in \mathcal{H}$. For any $\psi_N \in \mathcal{H}_N^{\text{sym}} := \bigotimes_{\text{sym}}^{N} \mathcal{H}$ with

$$\psi_N = \sum_{n_1,\ldots,n_N} \alpha_{n_1\ldots n_N} u_{n_1} \otimes \cdots \otimes u_{n_N},$$

define the operator $a(f) : \mathcal{H}_N^{\text{sym}} \to \mathcal{H}_{N-1}^{\text{sym}}$ by

$$a(f)\psi_N := \sqrt{N} \sum_{n_1,\ldots,n_N} \alpha_{n_1,\ldots,n_n} (f, u_{n_1}) u_{n_2} \otimes \cdots \otimes u_{n_N}$$

and similarly $a^*(f) : \mathcal{H}_N^{\text{sym}} \to \mathcal{H}_{N+1}^{\text{sym}}$ by

$$a^*(f)\psi_N := \frac{1}{\sqrt{N}} \sum_{n_1,\ldots,n_N} \alpha_{n_1,\ldots,n_N} f \otimes_{\text{sym}} u_{n_1} \otimes_{\text{sym}} \cdots \otimes_{\text{sym}} u_{n_N}.$$

For $f, g \in \mathcal{H}$ this definition implies the canonical commutation relation

$$[a(f), a^*(g)] = (f, g). \tag{1.22}$$

Stability of matter Earlier in this thesis it is mentioned that matter as it is experienced in everyday life or much simpler molecules are bound states of the electromagnetic interaction. Actually, it is not as simple as that. If there was only the electromagnetic interaction the system would not be stable. The reason why matter in this mathematical model is stable is that it consists of fermionic particles. The size of an atom is much larger than the size of an atomic nucleus precisely because electrons are fermions. Roughly speaking this means that only two electrons (one spin up and one spin down) can be in the same one-particle state. (For a discussion of the stability of matter refer to [35].)

The many particle limit The question of stability is connected to the question whether the thermodynamic limit exists. So, is the energy proportional to the particle number N or not? The mathematical model of N polarons that is considered is not stable, the energy is proportional to $-N^{7/5}$. This is connected with the fact that the typical length scales $L \propto N^{-1/5+\delta_L}$ and $l \propto N^{-2/5+\delta_l}$ tend to zero very quickly with increasing particle number N.

Nuclear matter The liquid drop model actually shows what happens if there is no antisymmetry condition in the mathematical model that keeps things apart. Atomic nuclei are much closer to each other. The typical distance is of a completely different order of magnitude in nuclear matter. Now the nuclear force is the attractive part in the energy while the Coulomb interaction describes the repulsive part of the energy.

Hartree state of N bosons Consider a system of N bosons with Hamiltonian

$$H_N := \sum_{i=1}^{N}(-\Delta_i) + \frac{1}{N-1}\sum_{1\le i<j\le N} V(x_i - x_j),$$

with some potential $V \in L^1_{\mathrm{loc}}(\mathbb{R}^3)$. A simple upper bound for the energy of the system is given by $(\psi, H_N\psi)$ for $\psi(x_1,\dots x_N) := \prod_{i=1}^N \varphi(x_i)$ where $\varphi \in H^2(\mathbb{R}^3)$. So all particles are in the same one particle state φ. Then, the energy is

$$(\psi, H_N\psi) = N(\varphi, -\Delta\varphi) + \frac{N}{2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} |\varphi(x)|^2 V(x-y)|\varphi(y)|^2 \,\mathrm{d}x\,\mathrm{d}y =: N\mathcal{E}_{\mathrm{HF}}(\varphi).$$

$\mathcal{E}_{\mathrm{HF}}$ is called *Hartree-Fock functional*. If there is Bose-Einstein condensation, then one actually has

$$\inf_{\psi\in D(H_N),\|\psi\|=1}(\psi, H_N\psi) = N \inf_{\varphi\in D(\mathcal{E}_{\mathrm{HF}}),\|\psi\|=1}\mathcal{E}_{\mathrm{HF}}(\varphi) + o(N).$$

So the leading order of the ground state energy of the large system is attained by all N particles being in the same one particle state. Bogolubov theory considers the excitations of states around this Hartree state to derive the second order ground state energy. This is explained in [34] in a very elegant setting.

The Bogolubov Hamiltonian In 1947 Bogolubov tried to explain superfluidity in terms of a Bose-Einstein gas [5]. Since he assumed the number of particles in the condensate $N_0 = a_0^* a_0$ to be much larger than the commutator $[a_0, a_0^*] := a_0 a_0^* - a_0^* a_0 = 1$ Bogolubov had the idea to replace the operators a_0^* and a_0 by the number $\sqrt{N_0}$ to calculate the ground state energy of the system.

Foldy used Bogolubov's method in 1961 to study a charged Bose gas in the limit of high densities [14]. Replacing $a_0^\#$ by $\sqrt{N_0}$ and neglecting all terms that do not contain exactly two $a_0^\# \in \{a_0, a_0^*\}$ Foldy diagonalized the resulting Hamiltonian to get an expression for the ground state energy of the system. In [36] Lieb and Solovej confirm Foldy's result rigorously. They derive a lower bound for the thermodynamic ground state energy of the quantum mechanical jellium model in the high density limit. Solovej also proves the corresponding upper bound in [46].

Following Bogolubov's approach, Lewin, Nam, Serfaty and Solovej show in [34] that in a very general setting the second order of the energy is described by the Bogolubov Hamiltonian if there is Bose-Einstein condensation. It is based on a unitary transform that basically replaces the operators a_0^* and a_0 by $\sqrt{N_0}$. See also the recent works [27, 40].

1.7 Large Polaron Systems and Bogolubov Theory

In a polar crystal there are phonons, i.e. modes of higher energy of atomic oscillations, and electrons interacting with these phonons [4]. Fröhlich describes this physical system in terms of a Hamiltonian containing the phonons as quantized fields and the the electron as a scalar wave function [21, 22]. An upper bound for the ground state energy is given by the non-linear Pekar-Tomasevich energy functional. Lieb and Thomas also prove a corresponding lower bound if only one polaron (i.e. one electron with the polarization that is induced in the ionic crystal) is considered in the limit of strong coupling $\alpha \to \infty$ [38]. A system of N Fröhlich polarons is considered by Frank, Lieb, Seiringer and Thomas in [19, 20].

In Chapter 4 a sharp lower bound for the ground state energy of a polaron system in the Pekar-Tomasevich approximation in the many particle limit is proven. Unlike the liquid drop model in which the thermodynamic limit does exist, for this polaron system the thermodynamic limit does not exist (at least in the case considered in this thesis that is $U = 1$). The ground state energy in fact is proportional to $N^{-7/5}$ as Benguria, Frank and Lieb show in [3]. They prove an upper bound which they conjecture to be sharp and a lower bound which differs by a factor of $2^{2/5}$. In this thesis it is shown that their conjecture is indeed true by proving the corresponding lower bound.

The Pekar-Tomasevich energy functional [42] is

$$\mathcal{E}_U^{(N)}[\psi] := \int_{(\mathbb{R}^3)^N} \left(\sum_{i=1}^N |\boldsymbol{\nabla}_i \psi|^2 + U \sum_{1 \le i < j \le N} \frac{|\psi|^2}{|x_i - x_j|} \right) \mathrm{d}x - D(\rho_\psi, \rho_\psi), \tag{1.23}$$

where the particle density is defined

$$\rho_\psi(z) := \sum_{i=1}^N \int \cdots \int_{(\mathbb{R}^3)^{N-1}} |\psi(x_1, \dots, x_{i-1}, z, x_{i+1}, \dots, x_N)|^2 \, \mathrm{d}x_1 \dots \mathrm{d}x_{i-1} \, \mathrm{d}x_{i+1} \dots \mathrm{d}x_N$$

and the Coulomb energy

$$D(\rho_1, \rho_2) := \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\overline{\rho_1(y)} \rho_2(z)}{|y - z|} \, \mathrm{d}y \, \mathrm{d}z \, .$$

The term $-D(\rho_\psi, \rho_\psi)$ is attractive. Minimizing the energy it favors polarons coming closer together. The sum $\sum_{1 \le i < j \le N} \frac{|\psi|^2}{|x_i - x_j|}$ is the Coulomb term which is repulsive. The relative strength of these two terms is described by the parameter U. (The Pekar-Tomasevich energy actually contains another parameter, the coupling constant α, which is eliminated by rescaling.)

Chapter 4 is concerned with the many particle limit $N \to \infty$ of the ground state energy

$$E_U^{(\mathrm{b})}(N) := \inf \left\{ \mathcal{E}_U^{(N)}[\psi] : \text{ symmetric } \psi \in H^1((\mathbb{R}^3)^N), \int_{(\mathbb{R}^3)^N} |\psi|^2 \, \mathrm{d}x = 1 \right\}, \tag{1.24}$$

in case $U = 1$. At this value for U there is a phase transition. For $U > 1$ the thermodynamic limit exists [18], whereas for $U < 1$ the bosonic ground state energy $E_U^{(\mathrm{b})}(N)$ goes as $-e_U^{(\mathrm{b})} N^3$ with a constant $e_U^{(\mathrm{b})}$ as Benguria and Bley show in [4]. Benguria, Frank and Lieb [3] prove in 2015 that for $U = 1$

$$-2^{2/5} A \leq \liminf_{N\to\infty} N^{-7/5} E_1^{(\mathrm{b})}(N) \leq \limsup_{N\to\infty} N^{-7/5} E_1^{(\mathrm{b})}(N) \leq -A,$$

for a certain $A > 0$ and conjecture the upper bound to be sharp. The following theorem shows that this is indeed true.

Theorem 1.7. *In the bosonic case with $U = 1$,*

$$\lim_{N\to\infty} N^{-7/5} E_1^{(\mathrm{b})}(N) = -A, \tag{1.25}$$

where

$$-A = \inf\left\{ \int_{\mathbb{R}^3} |\nabla \phi|^2 \,\mathrm{d}x - I_0 \int_{\mathbb{R}^3} |\phi|^{5/2} \,\mathrm{d}x : \ \phi \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |\phi|^2 \,\mathrm{d}x = 1 \right\}, \tag{1.26}$$

with

$$I_0 = \frac{2}{5}\left(\frac{2}{\pi}\right)^{1/4} \frac{\Gamma(3/4)}{\Gamma(5/4)} \approx 0.6. \tag{1.27}$$

The proof is based on a linearization of the Pekar-Tomasevich energy functional

$$\mathcal{E}_1^{(N)}[\psi] = \inf_\sigma (\psi, H_N \psi) \qquad \text{where } \psi \in H^1((\mathbb{R}^3)^N) \text{ and}$$
$$H_N = \sum_{j=1}^N (-\Delta_j) + \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|} - \sum_{j=1}^N \int_{\mathbb{R}^3} \frac{\sigma(y)}{|x_j - y|} \,\mathrm{d}y + \frac{1}{2} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\sigma(y)\sigma(z)}{|y-z|} \,\mathrm{d}y \,\mathrm{d}z\,.$$

Here, the infimum is taken over all $\sigma \in L^1(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\sigma(y)\sigma(z)}{|y-z|} \,\mathrm{d}y\,\mathrm{d}z < \infty$. Therefore, the techniques applied are those of Bose gases, in particular Bogolubov theory. The work is based on two remarkable papers by Lieb and Solovej on the one component and the two component charged Bose gases [36, 37].

The first paper mentioned is about the quantum mechanical jellium model that is the Hamiltonian H_N with $\sigma = \rho 1_{Q_L}$ for a constant $\rho > 0$. It has some similarity to the problem considered in this thesis because of the interaction of the wave function with a background of opposite charge. However, due to the fact that this background is chosen to be constant, the thermodynamic limit does exist.

The second paper is more similar to the problem considered in this thesis. In the two component charged Bose gas particles of charge -1 can accumulate around particles of charge 1. Similarly, in this thesis σ might be more concentrated at one spot than at another. This is why, for the two component charged Bose gas the thermodynamic limit does not exist, either. The system implodes as the particle number tends to infinity.

The large length scale There are two relevant length scales of this problem - exactly, the same es in [37]. Beginning with the system of N particles in the whole space $\mathbb{R}^3$, it is then considered in a cube $Q_L = (-L/2, L/2)^3$. As will be seen, the ground state in this cube is sub-additive in the particle number N. That is, (without specifying the energy E at the moment)

$$E(N_1 + N_2) \leq E(N_1) + E(N_2).$$

This is why the energy on the whole of $\mathbb{R}^3$ can be estimated from below by the energy of the system inside a cube of length scale $L \propto N^{-1/5+\delta_L}$ for some small $\delta_L > 0$. So L describes the size of the whole N particle system close to the ground state energy.

The small length scale As in [37] there is a small length scale $l \propto N^{-2/5+\delta_l}$ where there is local condensation, i.e. most particles in a cube of size l are in the constant state. This length scale l is where Bogolubov theory is applied. Heuristically, Bogolubov theory describes the second order energy. However, in this system it describes the leading order of the energy because there is local charge neutrality. In cubes of size l the difference of the local particle number density nl^{-3} and the background σ is of subleading order. Proving this is one of the challenges, but similar to what Lieb and Solovej have done one succeeds in doing so. Actually, there are two terms in the lower bound which are difficult to estimate, the non-neutrality term and the number of excitations.

The non-neutrality term is estimated by including it in the Bogolubov Hamiltonian that describes the leading order. The number of excitations is estimated using the method of localizing large matrices Lieb and Solovej developed in [36]. This is the major challenge that Lieb and Solovej overcome, not by getting a good estimate for the wave function itself, but by proving that there is a wave function of similar energy with a good estimate on the local number of excited particles.

Chapter 2

Ground State Energy of the Three Dimensional Liquid Drop Model

This chapter has been published [13]. It is joined work with Rupert Frank and Tobias König.

In this chapter Theorem 1.1 is proven which concerns the thermodynamic limit of the ground state energy in the dilute limit. It basically says that $\lim_{L\to\infty} E_{\rho,L}/L^3$ is given to leading order by the energy of an isolated nucleus that minimizes the energy $\mathcal{E}_0$ without a background.

As usual in statistical mechanics, the system is considered in a cube $Q_L = (-L/2, L/2)^3$ for $L > 0$. Allowed nuclear configurations are described by measurable sets $\Omega_{\rho,L} \subset Q_L$ that are electroneutral $|\Omega_{\rho,L}| = \rho L^3$ and their energy is

$$\mathcal{E}_{\rho,L}(\Omega_{\rho,L}) = \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L}\int_{Q_L} (1_{\Omega_{\rho,L}}(x) - \rho)\frac{1}{|x-y|}(1_{\Omega_{\rho,L}}(y) - \rho)\,\mathrm{d}x\,\mathrm{d}y\,. \tag{2.1}$$

The parameter $\rho \in (0,1)$ here describes the quotient between the electron and the nucleon charge density. The ground state energy is given by

$$E_{\rho,L} = \inf\left\{\mathcal{E}_{\rho,L}(\Omega) \,:\, \Omega \subset Q_L, |\Omega| = \rho L^3\right\}. \tag{2.2}$$

The main result of this chapter is the following theorem. It is crucial that this established uniformly in L.

Theorem 2.1 (Ground State Energy Asymptotics)**.** *There is a constant $C > 0$ such that the following bounds hold.*

(i) For all $\rho \in (0, \frac{1}{2}]$ and $L > 0$ such that $\rho^{1/3}L \geq C$, one has

$$\frac{E_{\rho,L}}{\rho L^3} \leq \frac{E_0(A^*)}{A^*} + C\rho^{1/3} + \frac{C}{\rho^{1/3}L}. \tag{2.3}$$

(ii) For all $\rho \in (0,1]$ and $L > 0$, one has

$$\frac{E_{\rho,L}}{\rho L^3} \geq \frac{E_0(A^*)}{A^*} - C\rho^{1/5}. \tag{2.4}$$

Remark 2.2. The bounds in Theorem 2.1 give the asymptotics of the energy for ρ close to 0. By a simple symmetry argument this theorem yields analogous asymptotics for ρ close to 1. Namely, for $\rho \in [\frac{1}{2}, 1)$ and $(1-\rho)^{1/3}L \geq C$, one has

$$-C(1-\rho)^{1/5} - \frac{6}{L} \leq \frac{E_{\rho,L}}{(1-\rho)L^3} - \frac{E(A^*)}{A^*} \leq C(1-\rho)^{1/3} + \frac{C}{(1-\rho)^{1/3}L}. \tag{2.5}$$

This follows from the fact that the energy fulfills for $\Omega \subset Q_L$

$$\mathcal{E}_{\rho,L}(\Omega) = \mathcal{E}_{1-\rho,L}(Q_L \backslash \Omega) - \Big(\mathcal{H}^2(\partial Q_L) - 2\mathcal{H}^2(\partial Q_L \cap \overline{\Omega})\Big),$$

where the closure of Ω is taken in the measure theoretic sense. The term in parentheses is bounded in absolute value by $6L^2$. Therefore, (2.5) follows from the bounds in Theorem 2.1.

Remark 2.3. The power $1/5$ of ρ in (2.4) is technical. It is an interesting question to decide whether the power $1/3$ in (2.3) is best possible. The assumption $\rho^{1/3}L \geq C$ and the corresponding remainder term in (2.3) are not severe restrictions in the thermodynamic limit and are imposed mainly for a simple statement.

Remark 2.4. Note that this result implies the main theorem stated in the introduction, namely Theorem 1.1 since in Chapter 3 the equality of the thermodynamic limit for Dirichlet, whole space, periodic and Neumann boundary conditions is deduced in Theorem 3.22.

Note that this result is valid independently of whether the energy-per-volume minimizer Ω^* of the functional $\mathcal{E}_0$ without background is a ball or not. This is particularly relevant for the proof of the upper bound (2.3). If Ω^* is a ball, or more generally, if the quadrupole moment of Ω^* vanishes, the proof of the upper bound (2.3) is straightforward. If the quadrupole moment of Ω^* does not vanish, one needs to distort the lattice to achieve the required cancellation in the long range behavior of the Coulomb potential.

The remainder of this chapter consists of three sections. Section 2.1 deals with the upper bound (2.3) of Theorem 2.1 under the additional assumption that the energy-per-volume minimizer Ω^* is a ball. In Section 2.2 the necessary changes are described to remove this assumption. Finally, Section 2.3 deals with the lower bound (2.4).

Throughout this chapter it is assumed $d = 3$.

2.1 Upper bound if Ω^* is a ball

The purpose of this and the next section is to prove the first statement of Theorem 2.1, which is restated here for convenience.

Proposition 2.5 (Upper Bound)**.** *There is a constant $C > 0$ such that, if $\rho^{1/3}L \geq C$ and $\rho \leq \frac{1}{2}$, one has*

$$\frac{E_{\rho,L}}{\rho L^3} \leq \frac{E_0(A^*)}{A^*} + C\rho^{1/3} + \frac{C}{\rho^{1/3}L}. \tag{2.6}$$

In order to not obscure the simple underlying idea, throughout this section make the additional assumption that the minimizer Ω^* of the whole space problem is a ball. As explained in the introduction, this is strongly conjectured to be the case. In the following Section 2.2 the technical modifications of the proof are explained to treat the case of general Ω^*.

Proof of Proposition 3.4 when Ω^* is a ball. For every pair (ρ, L) a suitable set $\Omega_{\rho,L}$ for $E_{\rho,L}$ is constructed. The idea is to take $\Omega_{\rho,L}$ to be given by a cubic lattice arrangement on Q_L of sets Ω^*. The period length $l > 0$ of the lattice will be chosen so that the requirement $|\Omega_{\rho,L}| = \rho L^3$ is fulfilled. Since each box of side length l should contain one copy of Ω^*, for the mass density to be equal to ρ, assume $\rho l^3 = A^*$, or equivalently

$$l = A^{*1/3}\rho^{-1/3}.$$

Let $\mathcal{C}_{\rho,L} := \{r \in l\mathbb{Z}^3 \,:\, Q_l(r) \subset Q_L\}$ be the set of lattice points r such that the cubes $Q_l(r)$ are fully contained in Q_L and let $N_{\rho,L} := \#\mathcal{C}_{\rho,L}$ denote the number of these cubes.

Define the set $\Omega_{\rho,L}$ to be the following disjoint union

$$\Omega_{\rho,L} := \bigcup_{r\in\mathcal{C}_{\rho,L}} (\lambda_{\rho,L} r + \lambda_{\rho,L}\Omega^*), \tag{2.7}$$

where the rescaling factor $\lambda_{\rho,L}$ is given by

$$\lambda^3_{\rho,L} = \frac{\rho L^3}{A^* N_{\rho,L}}. \tag{2.8}$$

Recall that it is assumed that Ω^* is a ball which is centered at the origin. Moreover, its radius is denoted by r_*.

Note that the union in (3.7) is disjoint since $\rho \le \frac{1}{2}$. (Indeed, one has $\frac{1}{2}l^3 \ge \rho l^3 = A^* = \frac{4\pi}{3}r_*^3$ and therefore, $l > 2r_*$.)

Informally, the construction of the set $\Omega_{\rho,L}$ can thus be described as follows. Fill Q_L with small boxes $Q_l(r)$ of side length l as full as possible, place a copy of Ω^* in the middle of each box and enlarge the whole configuration slightly by the factor $\lambda_{\rho,L}$.

The definition of $\lambda_{\rho,L}$ now ensures that the boxes $Q_{\lambda_{\rho,L}l}(\lambda_{\rho,L}r)$ cover Q_L completely and that the mass constraint

$$|\Omega_{\rho,L}| = N_{\rho,L}A^*\lambda^3_{\rho,L} = \rho L^3 \tag{2.9}$$

is fulfilled. Note also that with this choice, one even has *local neutrality* of $\Omega_{\rho,L}$ on every box $Q_{\lambda_{\rho,L}l}(\lambda_{\rho,L}r)$, i.e. for every $r \in \mathcal{C}_{\rho,L}$,

$$|\Omega_{\rho,L} \cap Q_{\lambda_{\rho,L}l}(\lambda_{\rho,L}r)| = \lambda^3_{\rho,L}A^* = \rho\lambda^3_{\rho,L}l^3 = \rho|Q_{\lambda_{\rho,L}l}(\lambda_{\rho,L}r)|. \tag{2.10}$$

Since the number of boundary boxes is of order $\frac{L^2}{l^2}$, it is easy to see that $N_{\rho,L}$ satisfies the bounds

$$\frac{L^3}{l^3} \ge N_{\rho,L} \ge \frac{L^3}{l^3} - C\frac{L^2}{l^2}, \tag{2.11}$$

for some $C > 0$ independent of ρ and L. From (2.8), one thus obtains the bound

$$1 \le \lambda_{\rho,L}^3 \le \frac{\rho L^3}{A^*\left(\frac{L^3}{l^3} - C\frac{L^2}{l^2}\right)} = \frac{\rho}{A^*(l^{-3} - CL^{-1}l^{-2})} = \frac{1}{1 - C\frac{l}{L}} \le 1 + C\frac{l}{L}, \tag{2.12}$$

and so, in particular, $\lim_{L\to\infty} \lambda_{\rho,L} = 1$.
In many situations below, to estimate subleading terms, the crude bound

$$1 \le \lambda_{\rho,L} \le 2, \tag{2.13}$$

is enough. It follows from (2.12) whenever $\frac{l}{L} = \frac{A^{*1/3}}{\rho^{1/3}L} \le \frac{1}{C}$.

The proof of the bound (3.6) consists in computing in three separate steps the self-energy, the near-field and the far-field interaction energy of the set $\Omega_{\rho,L}$. That is, the energy is expressed as the sum of three terms

$$\mathcal{E}_{\rho,L}(\Omega_{\rho,L}) = \mathcal{E}_{\rho,L}^{(\mathrm{self})} + \mathcal{E}_{\rho,L}^{(\mathrm{near})} + \mathcal{E}_{\rho,L}^{(\mathrm{far})}, \tag{2.14}$$

by partitioning the double integral from the interaction term of $\mathcal{E}_{\rho,L}$. To simplify notation, write

$$l = \lambda_{\rho,L} l, \quad r = \lambda_{\rho,L} r, \quad \text{and} \quad s = \lambda_{\rho,L} s \tag{2.15}$$

throughout the remaining proof. Define

$$\mathcal{E}_{\rho,L}^{(\mathrm{self})} := \mathrm{Per}(\Omega_{\rho,L}) + \sum_{r\in\mathcal{C}_{\rho,L}} \frac{1}{2}\int_{Q_l(r)}\int_{Q_l(r)} (1_{\Omega_{\rho,L}}(x) - \rho)\frac{1}{|x-y|}\Big(1_{\Omega_{\rho,L}}(y) - \rho\Big)\,\mathrm{d}x\,\mathrm{d}y\,, \tag{2.16}$$

and

$$\mathcal{E}_{\rho,L}^{(\mathrm{near})} := \sum_{(r,s)\in V_{\mathrm{near}}} \frac{1}{2}\int_{Q_l(r)}\int_{Q_l(s)} \Big(1_{\Omega_{\rho,L}}(x) - \rho\Big)\frac{1}{|x-y|}\Big(1_{\Omega_{\rho,L}}(y) - \rho\Big)\,\mathrm{d}x\,\mathrm{d}y\,, \tag{2.17}$$

where

$$V_{\mathrm{near}} := V_{\rho,L}^{(\mathrm{near})} := \Big\{(r,s) \in \mathcal{C}_{\rho,L} \times \mathcal{C}_{\rho,L} \text{ and } 1 \le |r-s|_\infty \le M\Big\}. \tag{2.18}$$

Here, $M \in \mathbb{N}$ is a number fixed throughout the proof (let us say $M = 10$).
Lastly, define

$$\mathcal{E}_{\rho,L}^{(\mathrm{far})} := \sum_{(r,s)\in V_{\mathrm{far}}} \frac{1}{2}\int_{Q_l(r)}\int_{Q_l(s)} \Big(1_{\Omega_{\rho,L}}(x) - \rho\Big)\frac{1}{|x-y|}\Big(1_{\Omega_{\rho,L}}(y) - \rho\Big)\,\mathrm{d}x\,\mathrm{d}y\,, \tag{2.19}$$

where

$$V_{\mathrm{far}} := V_{\rho,L}^{(\mathrm{far})} := \Big\{(r,s) \in \mathcal{C}_{\rho,L} \times \mathcal{C}_{\rho,L} \text{ and } |r-s|_\infty > M\Big\}. \tag{2.20}$$

Step 1: Self-Energy. Similar to l, write

$$\Omega^* = \lambda_{\rho,L}\Omega^* \tag{2.21}$$

here and throughout the remaining proof. Since $\Omega_{\rho,L}$ consists of $N_{\rho,L}$ disjoint copies of Ω^*, one has

$$\frac{\mathcal{E}^{(\mathrm{self})}_{\rho,L}}{\rho L^3} \le \frac{N_{\rho,L}}{\rho L^3}\left(\mathrm{Per}(\Omega^*) + \frac{1}{2}\int_{\Omega^*}\int_{\Omega^*}\frac{\mathrm{d}x\,\mathrm{d}y}{|x-y|} + \frac{\rho^2}{2}\int_{Q_l}\int_{Q_l}\frac{\mathrm{d}x\,\mathrm{d}y}{|x-y|}\right).$$

Since $\frac{N_{\rho,L}}{\rho L^3} = \frac{1}{A^*\lambda^3_{\rho,L}}$ by (2.9), one has

$$\begin{aligned}
\frac{\mathcal{E}^{(\mathrm{self})}_{\rho,L}}{\rho L^3} &\le \frac{1}{A^*}\left(\lambda^{-1}_{\rho,L}\,\mathrm{Per}(\Omega^*) + \frac{\lambda^2_{\rho,L}}{2}\int_{\Omega^*}\int_{\Omega^*}\frac{\mathrm{d}x\,\mathrm{d}y}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y + C\rho^2 l^5\right)\\
&\le \frac{E(A^*)}{A^*} + \frac{E(A^*)}{A^*}(\lambda^2_{\rho,L}-1) + C\rho^2 l^5\\
&\le \frac{E(A^*)}{A^*} + \frac{C}{\rho^{1/3}L} + C\rho^{1/3},
\end{aligned}$$

where the bound $\lambda^2_{\rho,L} - 1 \le C(\lambda^3_{\rho,L}-1) \le C\frac{l}{L} = C\frac{1}{\rho^{1/3}L}$ from (2.12) has been used for the last inequality. Moreover, recall $l \le \lambda_{\rho,L} l \le 2l$, from (2.13).

Step 2: Near Field Interaction. Due to the periodicity of $\Omega_{\rho,L}$, one has

$$\begin{aligned}
\frac{\mathcal{E}^{(\mathrm{near})}_{\rho,L}}{\rho L^3} &= \frac{1}{\rho L^3}\sum_{(r,s)\in V_{\mathrm{near}}}\frac{1}{2}\int_{Q_l(r)}\int_{Q_l(s)}\Big(1_{\Omega_{\rho,L}}(x)-\rho\Big)\frac{1}{|x-y|}\Big(1_{\Omega_{\rho,L}}(y)-\rho\Big)\,\mathrm{d}x\,\mathrm{d}y\\
&= \frac{1}{\rho L^3}\sum_{(r,s)\in V_{\mathrm{near}}}\frac{1}{2}\int_{Q_l}\int_{Q_l}(1_{\Omega^*}(x)-\rho)\frac{1}{|rl+x-sl-y|}(1_{\Omega^*}(y)-\rho)\,\mathrm{d}x\,\mathrm{d}y\\
&\le \frac{1}{\rho L^3}\sum_{(r,s)\in V_{\mathrm{near}}}\frac{1}{2}\left(\int_{\Omega^*}\int_{\Omega^*}\frac{1}{|rl+x-sl-y|}\,\mathrm{d}x\,\mathrm{d}y + \rho^2\int_{Q_l}\mathrm{d}x\int_{Q_l}\frac{1}{|y|}\,\mathrm{d}y\right),
\end{aligned} \tag{2.22}$$

since the integral over the symmetric-decreasing function $1/|\cdot|$ is largest on the cube centered at 0. This follows from the observation that three Steiner symmetrizations with respect to the coordinate directions e_1, e_2, e_3 transform any cube $Q_l(\mu)$ into the centered cube $Q_l(0)$. Furthermore, for every $r \ne s$ and $x, y \in \Omega^*$ one has

$$|rl + x - sl - y| \ge |r-s|l - |x-y| \ge \lambda_{\rho,L}(l - \mathrm{diam}(\Omega^*)) \ge l/C.$$

Here, it has been estimated $\frac{1}{2}l^3 \ge \rho l^3 = A^* = \frac{4\pi}{3}r_*^3$, which implies $l - 2r_* \ge l/C$. Therefore, the right hand side of (2.22) is bounded from above by

$$\frac{1}{\rho L^3}\sum_{r\in\mathcal{C}_{\rho,L}} M^3\left(\frac{C}{l} + C\rho^2 l^5\right) \le C\frac{L^3 l^{-3}}{\rho L^3}\left(l^{-1} + \rho^2 l^5\right) \le C\rho^{1/3}, \tag{2.23}$$

by bound (2.11). For the last inequality, recall the choice $\rho l^3 = |\Omega^*| = A^*$ and the bound $1 \le \lambda_{\rho,L} \le 2$ from (2.13).

Step 3: Far Field Interaction. Due to the periodicity of $\Omega_{\rho,L}$, one has

$$\begin{aligned}\mathcal{E}^{(\text{far})}_{\rho,L} &= \sum_{(r,s)\in V_{\text{far}}} \frac{1}{2}\int_{Q_l(r)}\int_{Q_l(s)} \Big(1_{\Omega_{\rho,L}}(x)-\rho\Big)\frac{1}{|x-y|}\Big(1_{\Omega_{\rho,L}}(y)-\rho\Big)\,\mathrm{d}x\,\mathrm{d}y \\ &= \sum_{(r,s)\in V_{\text{far}}} \frac{1}{2}\int_{Q_l}\int_{Q_l} (1_{\Omega^*}(x)-\rho)\frac{1}{|rl+x-sl-y|}(1_{\Omega^*}(y)-\rho)\,\mathrm{d}x\,\mathrm{d}y\,. \end{aligned} \tag{2.24}$$

The Taylor expansion

$$\frac{1}{|a-b|} = \frac{1}{|a|} + \frac{a\cdot b}{|a|^3} + \frac{1}{2}\frac{3(a\cdot b)^2 - a^2b^2}{|a|^5} + \mathcal{O}\bigg(\frac{|b|^3}{|a|^4}\bigg), \tag{2.25}$$

is valid for $a,b\in\mathbb{R}^3$ with $|a|\geq 4|b|$. Choose $a=(r-s)l+x$ and $b=y$.

By the assumption that $\Omega^*=B(0,r_*)$, the monopole, the dipole and the quadrupole moments of $1_{\Omega^*}-\rho 1_{Q_l}$ vanish.

That is, for all $a\in\mathbb{R}^3\backslash\{0\}$, the equation holds

$$\int_{\mathbb{R}^3} (1_{\Omega^*}(y)-\rho 1_{Q_l}(y))\bigg(\frac{1}{|a|}+\frac{a\cdot y}{|a|^3}+\frac{1}{2}\frac{3(a\cdot y)^2-a^2y^2}{|a|^5}\bigg)\,\mathrm{d}y = 0. \tag{2.26}$$

This follows from the neutrality condition (2.10) and the symmetries of a ball and a cube centered at 0. More precisely, the function $1_{\Omega^*}(y)-\rho 1_{Q_l}(y)$ is invariant under the reflection of one coordinate $y_i\mapsto -y_i$ as well as under the exchange of two coordinates y_i and y_j.

These symmetries cause the dipole, respectively the quadrupole moment to vanish. Note that this is one of only two places where the additional assumption $\Omega^*=B(0,r_*)$ enters in the proof. The other one is the fact that $\Omega^*=B(0,r_*)\subset Q_l$ for $\rho\leq\frac{1}{2}$ if $\rho l^3=|\Omega^*|$. For the necessary modifications to obtain an equation similar to (2.26) in the absence of the assumption $\Omega^*=B(0,r_*)$ refer to Section 2.2.

By (2.26), if one plugs in the expansion (2.25) and sets $a=(r-s)l+x$ and $b=y$, equation (2.24) is bounded from above by

$$\begin{aligned} &C\sum_{(r,s)\in V_{\text{far}}}\int_{Q_l}\int_{Q_l}|1_{\Omega^*}(x)-\rho|\frac{|y|^3}{|rl-sl+x|^4}|1_{\Omega^*}(y)-\rho|\,\mathrm{d}x\,\mathrm{d}y \\ &\leq C\sum_{(r,s)\in V_{\text{far}}}\int_{Q_l}\frac{1_{\Omega^*}(x)+\rho}{|(r-s)l+x|^4}\,\mathrm{d}x\int_{Q_l}(1_{\Omega^*}(y)+\rho)|y|^3\,\mathrm{d}y\,. \end{aligned} \tag{2.27}$$

Furthermore, $|x|\leq\sqrt{3}\,l/2$ for $x\in Q_l$. Since $|r-s|>M=10$, it follows $|(r-s)\tilde{l}+x|\geq \tilde{l}|r-s|-|x|\geq\frac{1}{2}\tilde{l}|r-s|$. Equation (2.27) can thus be estimated from above by

$$\begin{aligned} &C\sum_{(r,s)\in V_{\text{far}}}\frac{2^4}{l^4|r-s|^4}\int_{Q_l}(1_{\Omega^*}(x)+\rho)\,\mathrm{d}x\,\bigg(\int_{\Omega^*}|y|^3\,\mathrm{d}y+\rho\int_{Q_l}|y|^3\,\mathrm{d}y\bigg) \\ &\leq\frac{C}{l^4}\sum_{(r,s)\in V_{\text{far}}}\frac{1}{|r-s|^4}\Big(1+\rho l^3\Big)\Big(1+\rho l^6\Big)\leq Cl^{-1}(1+\rho l^3)(l^{-3}+\rho l^3)\sum_{(r,s)\in V_{\text{far}}}\frac{1}{|r-s|^4}, \end{aligned} \tag{2.28}$$

where again it is used $1 \leq \lambda_{\rho,L} \leq 2$, and thus, $l \leq l \leq 2l$, from (2.13).

Since $\rho l^3 = A^*$, it remains to evaluate the last sum over the set V_{far}. Recalling the bound on the number of boxes $N_{\rho,L} \leq \frac{L^3}{l^3}$, one has

$$\sum_{(r,s)\in V_{\text{far}}} \frac{1}{|r-s|^4} \leq \sum_{r\in\mathcal{C}_{\rho,L}} \sum_{\substack{s\in\mathbb{Z}^3\\ s\neq r}} \frac{1}{|r-s|^4} \leq \frac{L^3}{l^3} \sum_{s\in\mathbb{Z}^3\setminus\{0\}} \frac{1}{|s|^4} = C\rho L^3. \tag{2.29}$$

Putting together (2.24), (2.28) and (2.29) and using $\rho l^3 = A^*$, gives

$$\frac{1}{\rho L^3}\mathcal{E}^{(\text{far})}_{\rho,L} \leq Cl^{-1} = C\rho^{1/3}.$$

Step 4: Conclusion. Inserting the bounds proved in Steps 1-3 back into (2.14), one obtains

$$\frac{\mathcal{E}_{\rho,L}(\Omega_{\rho,L})}{\rho L^3} = \frac{\mathcal{E}^{(\text{self})}_{\rho,L} + \mathcal{E}^{(\text{near})}_{\rho,L} + \mathcal{E}^{(\text{far})}_{\rho,L}}{\rho L^3} \leq \frac{E(A^*)}{A^*} + C\rho^{1/3} + C\frac{1}{\rho^{1/3}L}.$$

The proof of Proposition 3.4 is therefore complete. □

2.2 Upper bound in the general case

Here, the necessary modifications are given to obtain the upper bound from Theorem 2.1 if one does not make any symmetry assumption on the energy-per-volume minimizer Ω^*.

In case $\rho > 1/C$, inequality (2.3) is equivalent to the bound

$$\frac{E_{\rho,L}}{\rho L^3} \leq C'.$$

To show this, it is not necessary to use minimizers in the construction of our test set $\Omega_{\rho,L}$. It suffices to consider balls of any fixed radius $r_* > 0$ arranged on a lattice just as it is done in the proof of Proposition 3.4. Therefore, assume

$$\rho \leq \frac{1}{C}.$$

The proof strategy of Theorem 2.1 in the absence of symmetry of Ω^* is identical to the one of the upper bound in Section 2.1. One constructs a competitor set made from energy-per-volume minimizers Ω^* arranged on a lattice. The difficulty one faces is that in proving the error bound on the far-field interaction term, one cannot invoke the symmetry of Ω^* to prove that the monopole, dipole and quadrupole moments vanish as in (2.26).

This difficulty can be resolved by fine-adjusting the parameters of the lattice. More precisely, it is shown that the analogue of (2.26) can still be achieved by considering a *suitably translated and rotated* copy of Ω^*, arranged on a *slightly distorted* lattice.

Notation. To deal with cuboids instead of cubes, it is necessary to introduce some appropriate notation. For $r \in \mathbb{R}^3$ and $\boldsymbol{l} \in \mathbb{R}^3$, define

$$Q_{\boldsymbol{l}}(r) := \{x \in \mathbb{R}^3 \,:\, |x_i - r_i| < l_i/2 \text{ for } i \in \{1,2,3\}\}, \tag{2.30}$$

and $Q_{\boldsymbol{l}} := Q_{\boldsymbol{l}}(0)$.

More generally, given $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \lambda_3) \in \mathbb{R}^3$ and $\Omega \subset \mathbb{R}^3$, define the 'inhomogeneous dilation' by $\boldsymbol{\lambda}$ of the set Ω to be $\boldsymbol{\lambda}\Omega := \{(\lambda_1 x_1, \lambda_2 x_2, \lambda_3 x_3) \,:\, x \in \Omega\}$. Observe that with these definitions, one has $\boldsymbol{\lambda} Q_L = Q_{L\boldsymbol{\lambda}}$. Both notations shall be used according to convenience.

It is intended to cover the cube Q_L with many copies of the cuboid of side lengths $\boldsymbol{l}$. Then, the parameter $r \in \boldsymbol{l}\mathbb{Z}^3$ simply counts those cuboids in each direction.

Furthermore, for $\Omega \subset \boldsymbol{\lambda} Q_L$, set

$$\mathcal{E}_{\rho,L,\boldsymbol{\lambda}}(\Omega) = \mathrm{Per}(\Omega) + \frac{1}{2}\int_{\boldsymbol{\lambda} Q_L}\int_{\boldsymbol{\lambda} Q_L} (1_\Omega(x) - \rho)|x-y|^{-1}(1_\Omega(y) - \rho)\,\mathrm{d}x\,\mathrm{d}y\,,$$

and define the corresponding ground state energy by

$$E_{\rho,L,\boldsymbol{\lambda}} = \inf\{\mathcal{E}_{\rho,L,\boldsymbol{\lambda}}(\Omega) \,:\, \Omega \subset \boldsymbol{\lambda} Q_L, |\Omega| = \rho|\boldsymbol{\lambda} Q_L|\}.$$

With this notation, one can prove the following two key lemmas.

Lemma 2.6 (Vanishing Multipole Moments)**.** *Let $\Omega \subset \mathbb{R}^3$ be a bounded set. Assume that two numbers $l_0 > 0$ and $\rho \in (0, \frac{1}{2}]$ are given such that $|\Omega| = \rho l_0^3$. If $\eta_0 := \frac{l_0}{\mathrm{diam}(\Omega)}$ is large enough, then there is an orthogonal matrix $U \in \mathbb{R}^{3\times 3}$, a translation vector $y \in \mathbb{R}^3$ and a scaling vector $\boldsymbol{l} = \boldsymbol{\lambda} l_0$ such that the set $\Omega_0 := U(\Omega + y)$ is contained in $Q_{\boldsymbol{l}}$ and satisfies*

$$\begin{aligned} 0 &= \int_{\mathbb{R}^3} (1_{\Omega_0}(x) - \rho 1_{Q_{\boldsymbol{l}}}(x))\,\mathrm{d}x = \int_{\mathbb{R}^3} x_i (1_{\Omega_0}(x) - \rho 1_{Q_{\boldsymbol{l}}}(x))\,\mathrm{d}x \\ &= \int_{\mathbb{R}^3} (3x_i x_j - \delta_{ij}|x|^2)(1_{\Omega_0}(x) - \rho 1_{Q_{\boldsymbol{l}}}(x))\,\mathrm{d}x \end{aligned}$$

for all $i, j \in \{1,2,3\}$. Furthermore, the scaling parameters $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \lambda_3)$ fulfill

$$\lambda_1\lambda_2\lambda_3 = 1 \qquad \text{and} \qquad |\lambda_i - 1| \le C\eta_0^{-2} \qquad (i = 1,2,3)$$

for a certain constant $C > 0$.

Remark 2.7. Since the proof below does not use the special form of 1_Ω as an indicator function, the statement of Lemma 2.6 remains true if one replaces 1_Ω by an arbitrary charge distribution $\tau \ge 0$, $\tau \in L^1(\mathbb{R}^3)$, with compact support.

Proof of Lemma 2.6. Let $\Omega \subset \mathbb{R}^3$ satisfy $|\Omega| = \rho l_0^3$. First, observe that since rotations and translations do not change the volume $|\Omega| = \rho l_0^3$, one always has

$$0 = \int_{\mathbb{R}^3} (1_{U(\Omega+y)}(x) - \rho 1_{Q_{\boldsymbol{l}}}(x))\,\mathrm{d}x\,,$$

as long as the constraint $\lambda_1\lambda_2\lambda_3 = 1$ is satisfied, which implies $|Q_{\boldsymbol{l}}| = l_0^3$.

Note that up to replacing Ω by its translate $\Omega + y$ for a suitable vector $y \in \mathbb{R}^3$, it can be achieved that

$$0 = \int_{\mathbb{R}^3} x_i(1_\Omega(x) - \rho 1_{Q_{\boldsymbol{l}}})\,\mathrm{d}x \qquad \text{for all } i = 1,2,3. \tag{2.31}$$

for every $\boldsymbol{l} \in \mathbb{R}^3$. Indeed, the cube $Q_{\boldsymbol{l}}$ is symmetric with respect to the coordinate planes and thus

$$0 = \rho \int_{\mathbb{R}^3} x_i 1_{Q_{\boldsymbol{l}}}(x)\,\mathrm{d}x\,.$$

Moreover, for $y \in \mathbb{R}^3$ one has

$$\int_{\mathbb{R}^3} 1_{\Omega+y}(x) x_i\,\mathrm{d}x = \int_{\mathbb{R}^3} 1_\Omega(x)(x_i + y_i)\,\mathrm{d}x = \int_\Omega x_i\,\mathrm{d}x + y_i|\Omega|,$$

Therefore, it suffices to set $y_i = -\frac{1}{|\Omega|}\int_\Omega x_i\,\mathrm{d}x$. Continue for simplicity to denote the translated version $\Omega + y$ which satisfies (2.31) by Ω. Note also that if Ω satisfies (2.31), then so does $U\Omega$, for any invertible matrix $U \in \mathbb{R}^{3\times 3}$.

It remains to ensure that the quadrupole moment vanishes by introducing an appropriate $U \in \mathbb{R}^{3\times 3}$ and $\boldsymbol{l} = \boldsymbol{\lambda} l_0 \in \mathbb{R}^3$. Since the quadrupole moment of Ω,

$$P = (P_{ij})_{i,j=1,2,3} \qquad \text{with} \qquad P_{ij} := \int_\Omega (3x_i x_j - \delta_{ij}|x|^2)\,\mathrm{d}x\,,$$

is a traceless symmetric 3×3-matrix with real entries, there is an orthogonal matrix $U \in \mathbb{R}^{3\times 3}$ and numbers $a, b \in \mathbb{R}$ such that

$$\begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & -a-b \end{bmatrix} = UPU^T = \int_\Omega (3(Ux)_i(Ux)_j - \delta_{ij}|Ux|^2)\,\mathrm{d}x = \int_{U\Omega} (3x_i x_j - \delta_{ij}|x|^2)\,\mathrm{d}x\,. \tag{2.32}$$

That is, up to replacing Ω by its rotated version $U\Omega =: \Omega_0$, whose monopole and dipole moments still vanish by the remarks made above, one can assume that its quadrupole moment is diagonal.

To make the quadrupole moment of $(1_{\Omega_0} - \rho 1_{Q_{\boldsymbol{l}}})$ vanish, it is thus necessary to find a cuboid $Q_{\boldsymbol{l}}$ of volume $|Q_{\boldsymbol{l}}| = l_0^3$ which contains Ω_0 and satisfies

$$\begin{aligned} \rho \int_{Q_{\boldsymbol{l}}} (3x_1^2 - |x|^2)\,\mathrm{d}x &= a, \\ \rho \int_{Q_{\boldsymbol{l}}} (3x_2^2 - |x|^2)\,\mathrm{d}x &= b. \end{aligned} \tag{2.33}$$

Setting $l_1 = \lambda_1 l_0$, $l_2 = \lambda_2 l_0$ and $l_3 = \lambda_3 l_0 = \frac{l_0}{\lambda_1\lambda_2}$ (by the volume constraint), then by rescaling and using the relation $|\Omega| = \rho l_0^3$, the system (2.33) is equivalent to

$$\begin{aligned} 2\lambda_1^2 - \lambda_2^2 - \frac{1}{\lambda_1^2\lambda_2^2} &= \frac{12}{|\Omega| l_0^2} a, \\ -\lambda_1^2 + 2\lambda_2^2 - \frac{1}{\lambda_1^2\lambda_2^2} &= \frac{12}{|\Omega| l_0^2} b. \end{aligned} \tag{2.34}$$

By adding these two equations, respectively subtracting them, one obtains the equations

$$\begin{aligned} \lambda_1^2 + \lambda_2^2 - \frac{2}{\lambda_1^2\lambda_2^2} &= \frac{12(a+b)}{|\Omega| l_0^2} =: 2c_1, \\ \lambda_1^2 - \lambda_2^2 &= \frac{4(a-b)}{|\Omega| l_0^2} =: 2c_2. \end{aligned} \tag{2.35}$$

Inserting the second equation of (2.35) into the first one and changing to the center of mass coordinate $X = (\lambda_1^2 + \lambda_2^2)/2$ gives the equation

$$X - \frac{1}{X^2 - c_2^2} = c_1, \tag{2.36}$$

which is equivalent to the cubic equation

$$p(X) := X^3 - c_1 X^2 - c_2^2 X - 1 + c_1 c_2^2 = 0. \tag{2.37}$$

It can be seen from (2.32) that $|a+b| \le 8\,\mathrm{diam}(\Omega_0)^2|\Omega_0|$. Therefore, the definition (2.35) of the c_i implies that $|c_i| < 48\,\mathrm{diam}(\Omega_0)^2 l_0^{-2}$. Thus, if $\eta_0 = \frac{l_0}{\mathrm{diam}(\Omega_0)}$ is large enough, the polynomial p will be very close to $X^3 - 1$. Since $X^3 - 1$ has exactly one complex zero close to 1 (namely 1), one can apply Rouché's theorem in a ball of radius $\sim \eta_0^{-2}$ around 1. Thus, there exists exactly one complex zero X_0 of p with $|X_0 - 1| \le C\eta_0^{-2}$. Since the coefficients of p are real, uniqueness of the zero implies that X_0 is in fact real.

One therefore gets solutions $\lambda_1, \lambda_2 > 0$ of (2.35) which satisfy

$$\begin{aligned} |\lambda_1 - 1| &= \frac{|\lambda_1^2 - 1|}{\lambda_1 + 1} = \frac{|X_0 + c_2 - 1|}{\lambda_1 + 1} \le C\eta_0^{-2}, \\ |\lambda_2 - 1| &= \frac{|\lambda_1^2 - 1|}{\lambda_1 + 1} = \frac{|X_0 - c_2 - 1|}{\lambda_1 + 1} \le C\eta_0^{-2}. \end{aligned}$$

Note that $\lambda_3 = 1/(\lambda_1\lambda_2)$ also fulfills $|\lambda_3 - 1| \le C\eta_0^{-2}$. Moreover, the fact that $\int_{\Omega_0} x_i \, dx = 0$ implies easily that $\Omega_0 \subset Q_{l_0}$ for every $l_0 \ge 2\,\mathrm{diam}(\Omega)$. This completes the proof of Lemma 2.6. □

The next lemma shows that for $\boldsymbol{\lambda}$ close to $(1,1,1)$, one can replace the ground state energy of Q_L by that of the cuboid $Q_{\boldsymbol{\lambda} L}$ with only a small error.

Lemma 2.8 (Approximating $E_{\rho,L}$ by a cuboid $E_{\rho,L,\boldsymbol{\lambda}}$)**.** *Suppose that $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \lambda_3)$ is such that $\lambda_1\lambda_2\lambda_3 = 1$ and assume that $\lambda_i \in [1-\delta, 1+\delta]$ for $i = 1, 2, 3$, for some $\delta \in [0,1]$. Then, one has*

$$\mathcal{E}_{\rho,L}(\Omega) \le (1 + C\delta)\mathcal{E}_{\rho,L,\boldsymbol{\lambda}}[\boldsymbol{\lambda}\Omega], \qquad \text{for all } \Omega \subset Q_L, \tag{2.38}$$

where $C > 0$ is a constant independent of δ, ρ, L and Ω. In particular, this implies

$$E_{\rho,L} \le (1 + C\delta)E_{\rho,L,\boldsymbol{\lambda}}. \tag{2.39}$$

Proof. Let $\Omega \subset Q_L$ arbitrary and consider, for $\boldsymbol{\lambda}$ as in the statement, the set $\boldsymbol{\lambda}\Omega$. Note that since $\lambda_1\lambda_2\lambda_3 = 1$, one has $|\boldsymbol{\lambda}\Omega| = |\Omega|$ and $|\boldsymbol{\lambda}Q_L| = |Q_L|$.

To prove (2.38), consider the perimeter and Coulomb terms separately. Assume for definiteness in the following that $\lambda_1 \leq \lambda_2 \leq \lambda_3$. Firstly, recall the definition

$$\mathrm{Per}(\Omega) = \sup\left\{ \int_\Omega \operatorname{div}\varphi(x)\,\mathrm{d}x \,:\, \varphi \in C_c^1(\mathbb{R}^3,\mathbb{R}^3), \|\varphi\|_\infty \leq 1 \right\}. \tag{2.40}$$

For any φ as in (2.40) and $\boldsymbol{\lambda} \in \mathbb{R}^3$ with $\lambda_1\lambda_2\lambda_3 = 1$, define the vector field $\varphi_{\boldsymbol{\lambda}} \in C_c^1(\mathbb{R}^3,\mathbb{R}^3)$ by setting its i-th component to be $\varphi_{\boldsymbol{\lambda},i}(x) = \lambda_i\varphi_i(\lambda_1^{-1}x_1, \lambda_2^{-1}x_2, \lambda_3^{-1}x_3)$. One easily checks that

$$\int_\Omega \operatorname{div}\varphi(x)\,\mathrm{d}x = \int_{\boldsymbol{\lambda}\Omega} \operatorname{div}\varphi_{\boldsymbol{\lambda}}(x)\,\mathrm{d}x = \|\varphi_{\boldsymbol{\lambda}}\|_\infty \int_{\boldsymbol{\lambda}\Omega} \operatorname{div}\frac{\varphi_{\boldsymbol{\lambda}}(x)}{\|\varphi_{\boldsymbol{\lambda}}\|_\infty}\,\mathrm{d}x\,. \tag{2.41}$$

Moreover, estimate

$$\|\varphi_{\boldsymbol{\lambda}}\|_\infty^2 = \sup_{x\in\mathbb{R}^3}\sum_{i=1}^3 \lambda_i^2\varphi_i^2(\lambda_1^{-1}x_1, \lambda_2^{-1}x_2, \lambda_3^{-1}x_3) \leq \lambda_3^2\|\varphi\|_\infty^2 \leq 1 + C\delta. \tag{2.42}$$

In view of the definition (2.40) of the perimeter, one can take the sup over all $\varphi \in C_c^1(\mathbb{R}^3,\mathbb{R}^3)$ with $\|\varphi\|_\infty \leq 1$ to obtain

$$\mathrm{Per}(\Omega) = \sup_\varphi \int_\Omega \operatorname{div}\varphi(x)\,\mathrm{d}x = \sup_\varphi \|\varphi_{\boldsymbol{\lambda}}\|_\infty \int_{\boldsymbol{\lambda}\Omega} \operatorname{div}\frac{\varphi_{\boldsymbol{\lambda}}(x)}{\|\varphi_{\boldsymbol{\lambda}}\|_\infty}\,\mathrm{d}x \leq (1 + C\delta)\,\mathrm{Per}(\boldsymbol{\lambda}\Omega), \tag{2.43}$$

where (2.42) is used for the last inequality.

To estimate the Coulomb term, it is convenient to pass to the Fourier representation. Set $f(x) := 1_\Omega(x) - \rho 1_{Q_L}(x)$, then

$$1_{\boldsymbol{\lambda}\Omega}(x) - \rho 1_{\boldsymbol{\lambda}Q_L}(x) = f(\lambda_1^{-1}x_1, \lambda_2^{-1}x_2, \lambda_3^{-1}x_3) =: f_{\boldsymbol{\lambda}}(x),$$

and one easily computes that $\mathfrak{F}[f_{\boldsymbol{\lambda}}](p) = \mathfrak{F}[f](\lambda_1 p_1, \lambda_2 p_2, \lambda_3 p_3)$. Therefore, it follows

$$\begin{aligned} \frac{1}{4\pi}\int_{Q_L}\int_{Q_L} \frac{(1_\Omega(x) - \rho)(1_\Omega(y) - \rho)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y &= \int_{\mathbb{R}^3} \frac{|\mathfrak{F}[f](p)|^2}{p^2}\,\mathrm{d}p = \int_{\mathbb{R}^3} \frac{|\mathfrak{F}[f_{\boldsymbol{\lambda}}](p)|^2}{\sum_{i=1}^3 \lambda_i^2 p_i^2}\,\mathrm{d}p \\ \leq \lambda_1^{-2}\int_{\mathbb{R}^3} \frac{|\mathfrak{F}[f_{\boldsymbol{\lambda}}](p)|^2}{p^2}\,\mathrm{d}p &\leq (1 + C\delta)\frac{1}{4\pi}\int_{\boldsymbol{\lambda}Q_L}\int_{\boldsymbol{\lambda}Q_L} \frac{(1_{\boldsymbol{\lambda}\Omega}(x) - \rho)(1_{\boldsymbol{\lambda}\Omega}(y) - \rho)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y\,. \end{aligned} \tag{2.44}$$

Combining estimates (2.43) and (2.44), the proof of (2.38) is complete.

The bound (2.39) on the ground state energy follows from (2.38) simply by taking the infimum over all $\Omega \subset Q_L$ with $|\Omega| = \rho L^3$. The proof of Lemma 2.8 is therefore complete. □

Using Lemmas 2.6 and 2.8, one can give the proof of the upper bound from Proposition 3.4 without assuming any symmetry on Ω^*. Since most parts are identical to the proof in Section 2.1, only the necessary modifications are given in the construction of the competitor set at the beginning of the proof.

Proof of Proposition 3.4 without symmetry of Ω^*. As in the proof given in Section 2.1, set $l_0 := A^{*1/3}\rho^{-1/3}$ to be the characteristic length of the small boxes. Let Ω^* be some set satisfying $|\Omega^*| = A^*$ and $\mathcal{E}[\Omega^*] = E(A^*)$. One may assume (up to changing Ω^* on a null-set) that $\operatorname{diam}(\Omega^*) < \infty$, see [31, Lemma 4.1] and [39, Lemma 4]. By Lemma 2.6, there are $U \in \mathbb{R}^{3\times 3}$ orthogonal, $y \in \mathbb{R}^3$ and $\boldsymbol{\lambda} \in \mathbb{R}^3$ with $|\lambda_i - 1| \le C l_0^{-2}$ and $\lambda_1\lambda_2\lambda_3 = 1$ such that setting $\boldsymbol{l} = \boldsymbol{\lambda} l_0$, the set $\Omega_0^* := U(\Omega^* + y)$ is contained in $Q_{\boldsymbol{l}}$ and satisfies

$$0 = \int_{\mathbb{R}^3} (1_{\Omega_0^*}(x) - \rho 1_{Q_{\boldsymbol{l}}})\,\mathrm{d}x = \int_{\mathbb{R}^3} x_i (1_{\Omega_0^*}(x) - \rho 1_{Q_{\boldsymbol{l}}})\,\mathrm{d}x = \int_{\mathbb{R}^3} (3x_i x_j - \delta_{ij}|x|^2)(1_{\Omega_0^*}(x) - \rho 1_{Q_{\boldsymbol{l}}})\,\mathrm{d}x\,. \tag{2.45}$$

By Lemma 2.8, one has

$$E_{\rho,L} \le (1 + C l_0^{-2}) E_{\rho,L,\boldsymbol{\lambda}} = (1 + C\rho^{2/3}) E_{\rho,L,\boldsymbol{\lambda}}. \tag{2.46}$$

To prove Proposition 3.4, it therefore suffices to prove the upper bound

$$\frac{E_{\rho,L,\boldsymbol{\lambda}}}{\rho L^3} \le \frac{E_0(A^*)}{A^*} + C\rho^{1/3} + \frac{C}{\rho^{1/3} L} \tag{2.47}$$

because the additional error term coming from the estimate (2.46) is subleading.

To prove (2.47), a competitor set is constructed by placing copies of the set Ω_0^* in boxes $Q_{\boldsymbol{l}}(r)$, $r \in \boldsymbol{l}\mathbb{Z}^3$. Let $\mathcal{C}_{\boldsymbol{l}} = \{r \in \boldsymbol{l}\mathbb{Z}^3 : Q_{\boldsymbol{l}}(r) \subset \boldsymbol{\lambda} Q_L\}$ be the set of lattice points r such that the cubes $Q_{\boldsymbol{l}}(r)$ are fully contained in $\boldsymbol{\lambda} Q_L$. Then, setting

$$\lambda_{\rho,L,\boldsymbol{\lambda}}^3 = \frac{\rho L^3}{A^* |\mathcal{C}_{\boldsymbol{l}}|}, \tag{2.48}$$

one obtains $\boldsymbol{\lambda} Q_L$ as a union of the boxes $Q_{\lambda_{\rho,L,\boldsymbol{\lambda}} l_0}(r)$. That is, the large box can exactly be covered by an integer number of small boxes. Therefore, define

$$\Omega_{\rho,L,\boldsymbol{\lambda}} = \bigcup_{r\in\mathcal{C}_{\boldsymbol{l}}} (\lambda_{\rho,L,\boldsymbol{\lambda}} \Omega_0^* + r).$$

Note that this definition fulfills the mass constraint

$$|\Omega_{\rho,L}| = |\mathcal{C}_{\boldsymbol{l}}| A^* \lambda_{\rho,L}^3 = \rho L^3. \tag{2.49}$$

The proof of Proposition 3.4 can now be finalized by following exactly the same steps as in Section 2.1, using the vanishing of the multipole moments from (2.45) in the bound on the far-field interaction. The remaining details are omitted. □

2.3 Lower bound

In this section, the proof of the lower bound from Theorem 2.1 is given. Again, the result is restated here for convenience.

Proposition 2.9 (Lower Bound)**.** *There is a constant $C > 0$ such that for all $\rho \in (0, 1]$, $L > 0$,*

$$\frac{E_{\rho,L}}{\rho L^3} \geq \frac{E_0(A^*)}{A^*} - C\rho^{1/5}. \tag{2.50}$$

The proof of Proposition 3.5 is based on reducing the problem to a smaller length scale $1 \ll R \ll L$.

Define the Yukawa potential

$$Y_\omega(x) = \frac{\mathrm{e}^{-\omega|x|}}{|x|} \qquad \text{for} \quad x \in \mathbb{R}^3 \quad \text{and} \quad \omega > 0.$$

Using Y_ω, the interaction part of $\mathcal{E}_{\rho,L}(\Omega)$ can be bounded from below as follows.

Lemma 2.10 (Lower bound on the interaction term)**.** *There is $C > 0$ such that for all $L > 0$, all $\rho \in [0, 1]$, all $\omega > 0$ and all $\Omega \subset Q_L$, one has*

$$\begin{aligned} &\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} (1_\Omega(x) - \rho 1_{Q_L}(x)) \frac{1}{|x-y|} (1_\Omega(y) - \rho 1_{Q_L}(y))\,\mathrm{d}x\,\mathrm{d}y \\ &\geq \int_{\mathbb{R}^3} 1_\Omega(x) Y_\omega(x-y)\, 1_\Omega(y)\,\mathrm{d}x\,\mathrm{d}y - C|\Omega|\rho\omega^{-2}. \end{aligned}$$

Proof. First, one can estimate

$$\begin{aligned} &\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} (1_\Omega(x) - \rho 1_{Q_L}(x)) \frac{1}{|x-y|} (1_\Omega(y) - \rho 1_{Q_L}(y))\,\mathrm{d}x\,\mathrm{d}y \\ &\geq \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} (1_\Omega(x) - \rho 1_{Q_L}(x)) Y_\omega(x-y) (1_\Omega(y) - \rho 1_{Q_L}(y))\,\mathrm{d}x\,\mathrm{d}y\,, \end{aligned}$$

because $\mathfrak{F}[\frac{1}{|x|}] = \sqrt{\frac{2}{\pi}}\frac{1}{|k|^2} \geq \sqrt{\frac{2}{\pi}}\frac{1}{|k|^2+\omega^2} = \mathfrak{F}[Y_\omega](k)$, where the Fourier transform is denoted by $\mathfrak{F}[f](k) := (2\pi)^{-3/2}\int_{\mathbb{R}^3} f(x)e^{-ikx}\,\mathrm{d}x$ for $f \in L^1(\mathbb{R}^3)$. Next,

$$\begin{aligned} &\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} (1_\Omega(x) - \rho 1_{Q_L}(x))\, Y_\omega(x-y)\, (1_\Omega(y) - \rho 1_{Q_L}(y))\,\mathrm{d}x\,\mathrm{d}y \\ &\geq \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} 1_\Omega(x)\, Y_\omega(x-y)\, 1_\Omega(y)\,\mathrm{d}x\,\mathrm{d}y - 2\rho\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} 1_\Omega(x) Y_\omega(x-y) 1_{Q_L}(y)\,\mathrm{d}x\,\mathrm{d}y \\ &\geq \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} 1_\Omega(x) Y_\omega(x-y)\, 1_\Omega(y)\,\mathrm{d}x\,\mathrm{d}y - C|\Omega|\rho\omega^{-2}, \end{aligned} \tag{2.51}$$

where it is bounded $\int_{Q_L} Y_\omega(x-y)\,\mathrm{d}y \leq \int_{\mathbb{R}^3} \frac{e^{-\omega|y|}}{|y|}\,\mathrm{d}y \leq C\omega^{-2}$. □

One also needs to control the behavior of the perimeter term under localization of $\Omega \subset Q_L$ to smaller boxes. The following lemma is useful for this purpose.

Lemma 2.11 (Localization of the perimeter term)**.** *Let $\Omega \subset \mathbb{R}^3$ have finite perimeter. Then for every $R > 0$,*

$$\mathrm{Per}(\Omega) \geq \sum_{m\in\mathbb{Z}^3}\int_{Q_1} \mathrm{Per}(\Omega \cap Q_R(m+\xi))\,\mathrm{d}\xi - \frac{6|\Omega|}{R}.$$

Proof. In every box, the boundary of $\Omega \cap Q_R(m+\xi)$ consists of two parts: the portion of $\partial\Omega$ lying inside $Q_R(m+\xi)$, and the portion of Ω intersecting $\partial Q_R(m+\xi)$, which is added by partitioning Ω into boxes. One therefore has that

$$\begin{aligned}
&\sum_{m\in\mathbb{Z}^3}\int_{Q_1}\mathrm{Per}(\Omega\cap Q_R(m+\xi))\,\mathrm{d}\xi \\
&\leq \int_{Q_1}\sum_{m\in\mathbb{Z}^3}\mathcal{H}^2(\partial\Omega\cap Q_R(m+\xi))\,\mathrm{d}\xi + \int_{Q_1}\sum_{m\in\mathbb{Z}^3}\mathcal{H}^2(\Omega\cap\partial Q_R(m+\xi))\,\mathrm{d}\xi \\
&\leq \mathrm{Per}(\Omega) + \int_{Q_1}\sum_{m\in\mathbb{Z}^3}\mathcal{H}^2(\Omega\cap\partial Q_R(m+\xi))\,\mathrm{d}\xi\,. \qquad (2.52)
\end{aligned}$$

Here, $\mathcal{H}^2$ denotes two-dimensional Hausdorff measure. It remains to evaluate the second term in (3.10). Since all sets appearing there are subsets of faces of cubes, decompose

$$\bigcup_{m\in\mathbb{Z}^3}\Omega\cap\partial Q_R(m+\xi) = \bigcup_{i=1}^{3}\bigcup_{l\in\mathbb{Z}}\Omega\cap\Big\{x\in\mathbb{R}^3\colon\ x_i = R\Big(l+\frac{1}{2}+\xi_i\Big)\Big\},$$

i.e. 'slices' of $\Omega\cap\partial Q_R(m+\xi)$ are distinguished according to the coordinate hyperplane they are parallel to. Note that $\mathcal{H}^2$-almost every point in one hyperplane is contained in the boundary of exactly two cubes adjacent to the plane. Thus, the union $\bigcup_{i=1}^3$ is disjoint up to an $\mathcal{H}^2$-null set and one obtains

$$\int_{Q_1}\sum_{m\in\mathbb{Z}^3}\mathcal{H}^2(\Omega\cap\partial Q_R(m+\xi))\,\mathrm{d}\xi = 2\sum_{i=1}^{3}\int_{[-1/2,1/2]^3}\mathrm{d}\xi_1\,\mathrm{d}\xi_2\,\mathrm{d}\xi_3\sum_{l\in\mathbb{Z}}\mathcal{H}^2(\Omega\cap\{x_i=R(l+1/2+\xi_i)\}).$$

The integrand on the right hand side only depends on *one* of the ξ_i. One can therefore do the $\mathrm{d}\xi_j$-integrations with $j\neq i$ to find that

$$\begin{aligned}
\int_{Q_1}\sum_{m\in\mathbb{Z}^3}\mathcal{H}^2(\Omega\cap\partial Q_R(m+\xi))\,\mathrm{d}\xi &= 2\sum_{i=1}^{3}\int_{-1/2}^{1/2}\sum_{l\in\mathbb{Z}}\mathcal{H}^2(\Omega\cap\{x_i=R(l+1/2+\xi_i)\})\,\mathrm{d}\xi_i \\
= 2\sum_{i=1}^{3}\int_{\mathbb{R}}\mathcal{H}^2(\Omega\cap\{x_i=R\xi_i\})\,\mathrm{d}\xi_i &= \frac{2}{R}\sum_{i=1}^{3}\int_{\mathbb{R}}\mathcal{H}^2(\Omega\cap\{x_i=\xi_i\})\,\mathrm{d}\xi_i = \frac{6|\Omega|}{R}
\end{aligned}$$

by Fubini's theorem. Plugging this in (3.10) completes the proof of Lemma 3.7. □

In the next lemma the estimates above are combined to obtain the crucial lower bound on the energy in terms of the auxiliary parameters R and ω.

Lemma 2.12. *For every $\Omega\subset Q_L$ with $|\Omega|>0$ and every $R>0$, one has that*

$$\frac{\mathcal{E}_{\rho,L}(\Omega)}{|\Omega|} \geq e^{-\sqrt{3}\omega R}\frac{E_0(A^*)}{A^*} - C\rho\omega^{-2} - \frac{6}{R}.$$

Proof. Let $\Omega \subset Q_L$ and $R > 0$. Ω is the (finite) disjoint union

$$\Omega = \bigcup_{m\in\mathbb{Z}^3} \Big(\Omega \cap Q_R(m+\xi_0)\Big) =: \bigcup_{m\in\mathbb{Z}^3} \Omega^{(m)} \tag{2.53}$$

for some $\xi_0 \in Q_1$ to be chosen below. Note that the choice of $\Omega^{(m)}$ in (3.11) ensures that $\operatorname{diam}(\Omega^{(m)}) \le \sqrt{3}R$.

Then, starting from Lemma 3.6 and dropping the interactions between different boxes, one can estimate the energy from below as follows.

$$\begin{aligned}\mathcal{E}_{\rho,L}(\Omega) &\ge \sum_{m\in\mathbb{Z}^3} \left(\operatorname{Per}(\Omega^{(m)}) + e^{-\omega\sqrt{3}R}\frac{1}{2}\iint_{\Omega^{(m)}\times\Omega^{(m)}} \frac{\mathrm{d}x\,\mathrm{d}y}{|x-y|}\right) + \mathcal{P}_R - C|\Omega|\rho\omega^{-2}\\ &\ge e^{-\sqrt{3}\omega R}\sum_{m\in\mathbb{Z}^3} \mathcal{E}(\Omega^{(m)}) + \mathcal{P}_R - C|\Omega|\rho\omega^{-2}\end{aligned} \tag{2.54}$$

with the perimeter error term $\mathcal{P}_R := \operatorname{Per}(\Omega) - \sum_{m\in\mathbb{Z}} \operatorname{Per}(\Omega^{(m)})$.

For every $m \in \mathbb{Z}^3$ with $|\Omega^{(m)}| > 0$, one has $\frac{\mathcal{E}_0(\Omega^{(m)})}{|\Omega^{(m)}|} \ge \frac{E_0(A^*)}{A^*}$, and therefore

$$\sum_{m\in\mathbb{Z}^3} \mathcal{E}_0(\Omega^{(m)}) = \sum_{m\in\mathbb{Z}^3, |\Omega^{(m)}|>0} \frac{\mathcal{E}_0(\Omega^{(m)})}{|\Omega^{(m)}|}|\Omega^{(m)}| \ge \frac{E_0(A^*)}{A^*}\sum_{m\in\mathbb{Z}^3} |\Omega^{(m)}| = |\Omega|\frac{E_0(A^*)}{A^*}. \tag{2.55}$$

Together with (2.55), the lower bound (3.12) implies

$$\mathcal{E}_{\rho,L}(\Omega) \ge e^{-\sqrt{3}\omega R}\frac{E(A^*)}{A^*}|\Omega| + \mathcal{P}_R - C|\Omega|\rho\omega^{-2}. \tag{2.56}$$

To bound the perimeter error $\mathcal{P}_R$ appropriately, recall from Lemma 3.7 that the averaged estimate holds

$$\int_{Q_1} \left(\sum_{m\in\mathbb{Z}^3} \operatorname{Per}(\Omega \cap Q_R(m+\xi))\right) \mathrm{d}\xi \le \operatorname{Per}(\Omega) + \frac{6|\Omega|}{R}, \tag{2.57}$$

and therefore there exists $\xi_0 \in Q_1$ depending on Ω such that

$$\sum_{m\in\mathbb{Z}^3} \operatorname{Per}(\Omega \cap Q_R(m+\xi_0)) \le \operatorname{Per}(\Omega) + \frac{6|\Omega|}{R}. \tag{2.58}$$

With this choice of ξ_0, one arrives at the bound

$$\mathcal{P}_R = \operatorname{Per}(\Omega) - \sum_{m\in\mathbb{Z}} \operatorname{Per}(\Omega^{(m)}) \ge -\frac{6|\Omega|}{R}. \tag{2.59}$$

Combining (2.56) and (3.15) and dividing by $|\Omega|$, the statement of Lemma 2.12 follows. □

It only remains to minimize the errors of the lower bound to the ground state energy $E_{\rho,L}$.

Proof of Proposition 3.5. Recalling that $|\Omega| = \rho L^3$, by Lemma 2.12 one has

$$\frac{E_{\rho,L}}{\rho L^3} \geq e^{-\sqrt{3}\omega R} \frac{E_0(A^*)}{A^*} - C\rho\omega^{-2} - \frac{6}{R}. \tag{2.60}$$

Since $e^{-x} \geq 1 - x$, from (2.60) it is obtained

$$\begin{aligned} \frac{E_{\rho,L}}{\rho L^3} &\geq \left(1 - \sqrt{3}\omega R\right) \frac{E_0(A^*)}{A^*} - C\rho\omega^{-2} - \frac{C}{R} \\ &\geq \frac{E_0(A^*)}{A^*} - C\omega R - \frac{C}{R} - C\rho\omega^{-2}. \end{aligned}$$

Optimizing first in R, take $R = \omega^{-1/2}$. With that choice, one has the inequality

$$\frac{E_{\rho,L}}{\rho L^3} \geq \frac{E_0(A^*)}{A^*} - C\omega^{1/2} - C\rho\omega^{-2}.$$

Optimizing in ω gives $\omega = \rho^{2/5}$, and thus, one gets

$$\frac{E_{\rho,L}}{\rho L^3} \geq \frac{E_0(A^*)}{A^*} - C\rho^{1/5}.$$

The proof of Proposition 3.5 is now complete. □

Chapter 3

Further Results on the Liquid Drop Model

3.1 The Ground State Energy in Two Dimensions

Similar to what has been done in the previous chapter in three dimensions the ground state energy per unit volume is considered for $d = 2$ in this section and Theorem 1.3 is proven. The upper bound is formulated such that one might conjecture that it is sharp up to the second order for small $\rho > 0$. The lower bound that is derived reproduces the order of this conjectured second order asymptotics. It is only sharp to leading order, though. The proof gives insight into how most connected components (droplets) behave in the dilute limit. Most of them approach a certain mass and their shape approaches the shape of a disk.

Recall that for $L > 0$ the liquid drop model energy of a measurable set $\Omega_{\rho,L} \subset Q_L = (-L/2, L/2)^2$ with $|\Omega_{\rho,L}| = \rho L^2$ is given in $d = 2$ by

$$\mathcal{E}_{\rho,L}(\Omega_{\rho,L}) = \operatorname{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L}\int_{Q_L} (1_{\Omega_{\rho,L}}(x) - \rho) \ln \frac{1}{|x-y|} (1_{\Omega_{\rho,L}}(y) - \rho) \,\mathrm{d}x \,\mathrm{d}y \,. \tag{3.1}$$

The parameter $\rho \in (0, 1)$ describes the quotient between the electron and the nucleon charge density. The corresponding ground state energy is denoted by

$$E_{\rho,L} = \inf \left\{ \mathcal{E}_{\rho,L}(\Omega) \,:\, \Omega \subset Q_L, |\Omega| = \rho L^2 \right\}. \tag{3.2}$$

Note that the constraint $|\Omega_{\rho,L}| = \rho L^2$ means that only neutral configurations are considered. As in the three dimensional case, the behavior of the energy per unit volume $E_{\rho,L}/L^2$ is considered in the dilute limit ρ tending to zero. Since the thermodynamic limit $L \to \infty$ is taken first and then, the dilute limit $\rho \to 0$, one might assume that L is arbitrarily large compared to $1/\rho$.

The upper bound derived in this section is stated in terms of the ground state energy of jellium.

$$e_{\text{Jellium}} := \lim_{L\to\infty} \frac{1}{L^2} \inf_{(x_1,\dots,x_N)\in\mathcal{A}_{\text{Jellium}}(L)} \Bigg(\sum_{1\le i<j\le N} \ln \frac{1}{|x_i - x_j|} - \sum_{i=1}^{N} \int_{Q_L} \ln \frac{1}{|x_i - z|}\,\mathrm{d}z + \frac{1}{2}\int_{Q_L}\int_{Q_L} \ln\frac{1}{|z-\tilde z|}\,\mathrm{d}z\,\mathrm{d}\tilde z \Bigg). \tag{3.3}$$

The set of admissible configurations is

$$\mathcal{A}_{\text{Jellium}}(L) := \Big\{ (x_1,\dots,x_N) \in (Q_L)^N : N = L^2, \forall i,j \in \{1,\dots,N\} : x_i \ne x_j \text{ for } i \ne j \text{ and } \operatorname{dist}(x_i, Q_L) \ge \sqrt{\rho/\pi} \Big\}.$$

Note that for technical reasons it is assumed that there is a tiny distance between each point x_i in the configuration and the boundary. (Compare how Armstrong and Serfaty enforce a distance to the boundary in the jellium model in Section 2.3 of [2] by introducing an additional potential in the energy.)

The main result of this section is the following theorem.

Theorem 3.1 (Ground State Energy Asymptotics)**.** *There is a constant $C > 0$ such that the following bounds hold.*

(i) For all $\rho \in (0, \frac{1}{C}]$ and $L > 0$, one has

$$\frac{E_{\rho,L}}{\rho L^2} \le 3\left(\frac{\pi}{4}\ln\frac{1}{\rho} + \frac{\pi}{4}\left(\ln\pi + \frac{1}{2}\right) + \pi\, e_{\text{Jellium}} + \frac{\pi\rho}{4}\right)^{1/3} + R_{L/l}, \tag{3.4}$$

where $R_{L/l} \to 0$ as $L \to \infty$.

(ii) For all $\rho \in (0, \frac{1}{C}]$ and $L > 0$, one has

$$\frac{E_{\rho,L}}{\rho L^2} \ge 3\left(\frac{\pi}{4}\ln\frac{1}{\rho}\right)^{1/3} - \frac{C}{(\ln\frac{1}{\rho})^{2/3}}. \tag{3.5}$$

Note that the dependence of the error estimates on the density ρ is explicit. In particular, it is not necessary to couple the dilute limit to the thermodynamic limit as it is sometimes done in the literature (e.g. [25]). This is very sensible from the perspective of physics. On a macroscopic scale L the particle number N is so large that the limit $N \to \infty$ seems to be a reasonable approximation. Regarding the density ρ, however, one cannot really assume $\rho = 0$ because then there are neither particles nor matter. So $\rho \gg \frac{1}{L}$ is physically a very sensible assumption.

To formulate the result about the droplets, let $\Omega_{\rho,L} \subset Q_L$ be a minimizer of $\mathcal{E}_{\rho,L}$ over all measurable $\Omega \subset Q_L$ such that $|\Omega| = \rho L^2$. In the proof of the lower bound it is shown that one may assume $\Omega_{\rho,L} = \bigcup_{j\in J} \Omega_j$ with $\Omega_{j_1} \cap \Omega_{j_2} = \emptyset$ for $j_1 \neq j_2$, Ω_j connected, $\mathrm{diam}(\Omega_j) \leq C(\ln \frac{1}{\rho})^{2/3}$ for all $j \in J$ and

$$\mathrm{Per}(\Omega_{\rho,L}) \geq \sum_{j\in J} \mathrm{Per}(\Omega_j) - \frac{C|\Omega_{\rho,L}|}{(\ln \frac{1}{\rho})^{2/3}}.$$

Corollary 3.2 (Mass and Shape of Droplets)**.** *Define* $\kappa := \frac{2^{4/3}\pi^{1/3}}{(\ln \frac{1}{\rho})^{2/3}}$*. For* $\epsilon > 0$ *let*

$$J_\epsilon := \left\{ j \in J : \left(\frac{|\Omega_j|}{\kappa} - 1 \right)^2 > \epsilon \quad \text{or} \quad \frac{\mathrm{Per}(\Omega_j)}{\sqrt{4\pi|\Omega_j|}} - 1 > \epsilon \right\}.$$

Define the total mass of all droplets which are not close to the optimal disk $m_\epsilon := \sum_{j\in J_\epsilon} |\Omega_j|$*. Then, for* $\rho \in (0, \frac{1}{C})$

$$\frac{m_\epsilon}{|\Omega_{\rho,L}|} \leq \frac{C}{\epsilon \ln \frac{1}{\rho}}.$$

Remark 3.3. By the quantitative isoperimetric inequality $\frac{\mathrm{Per}(\Omega_j)}{\sqrt{4\pi|\Omega_j|}} - 1$ is a measure of how close Ω_j is to the shape a disk.

The next two subsections are concerned with the proof of Theorem 3.1. The corollary on the mass and the shape of the droplets is proven in the final part of this section.

Throughout this section it is assumed $d = 2$.

3.1.1 Upper Bound on the Ground State Energy

The purpose of this section is to prove the first statement of Theorem 2.1, which is restated here for convenience.

Proposition 3.4 (Upper Bound)**.** *There is a constant* $C > 0$ *such that, if* $\rho \leq \frac{1}{C}$*, one has*

$$\frac{E_{\rho,L}}{\rho L^2} \leq 3\left(\frac{\pi}{4} \ln \frac{1}{\rho} + \frac{\pi}{4}\left(\ln \pi + \frac{1}{2}\right) + \pi\, e_{\mathrm{Jellium}} + \frac{\pi\rho}{4}\right)^{1/3} + R_{L/l}, \tag{3.6}$$

where $R_{L/l} \to 0$ *as* $L \to \infty$.

Proof. To prove Proposition 3.4, construct, for every pair (ρ, L), a suitable state $\Omega_{\rho,L}$ and evaluate the corresponding energy $\mathcal{E}_{\rho,L}(\Omega_{\rho,L})$. The idea is to place discs $B(0, lR)$ on points $lx_1, \ldots, lx_N \in Q_L$ with $l > 0$. To make this precise, let $\mathcal{C}_{\rho,L} := \{x_1, \ldots, x_N\} \subset Q_{L/l}$ be a discrete set such that

(i) $\mathrm{dist}(\mathcal{C}_{\rho,L}, \partial Q_{L/l}) \geq R$,

(ii) $|x - y| \geq 2R$ for $x, y \in \mathcal{C}_{\rho,L}, x \neq y$

(iii) $N := \#\mathcal{C}_{\rho,L} = \frac{L^2}{l^2}$.

Now, define the trial state $\Omega_{\rho,L}$ to be the union

$$\Omega_{\rho,L} := \bigcup_{x\in\mathcal{C}_{\rho,L}} (lx + lB_R) \tag{3.7}$$

and impose neutrality, i.e.

$$\rho = \pi R^2.$$

Then,

$$|\Omega_{\rho,L}| = \sum_{x\in\mathcal{C}_{\rho,L}} |lB_R| = Nl^2\pi R^2 = Nl^2\rho = \rho L^2.$$

One has

$$\begin{aligned}
\mathcal{E}_{\rho,L}(\Omega_{\rho,L}) &= \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L}\int_{Q_L}(1_{\Omega_{\rho,L}}(z)-\rho)\ln\frac{1}{|z-\tilde{z}|}(1_{\Omega_{\rho,L}}(\tilde{z})-\rho)\,\mathrm{d}z\,\mathrm{d}\tilde{z} \\
&= N2\pi Rl + \frac{l^4}{2}\int_{Q_{L/l}}\int_{Q_{L/l}}\left(\sum_{x\in\mathcal{C}_{\rho,L}} 1_{x+B_R}(z)-\rho\right)\ln\frac{1}{|z-\tilde{z}|}\left(\sum_{y\in\mathcal{C}_{\rho,L}} 1_{y+B_R}(\tilde{z})-\rho\right)\mathrm{d}z\,\mathrm{d}\tilde{z} \\
&= N2\pi Rl + \sum_{x\in\mathcal{C}_{\rho,L}}\frac{l^4}{2}\int_{x+B_R}\int_{x+B_R}\ln\frac{1}{|z-\tilde{z}|}\,\mathrm{d}z\,\mathrm{d}\tilde{z} \\
&\quad + \sum_{x,y\in\mathcal{C}_{\rho,L},x\neq y}\frac{l^4}{2}\int_{x+B_R}\int_{y+B_R}\ln\frac{1}{|z-\tilde{z}|}\,\mathrm{d}z\,\mathrm{d}\tilde{z} \\
&\quad - \sum_{x\in\mathcal{C}_{\rho,L}}\rho l^4\int_{x+B_R}\int_{Q_{L/l}}\ln\frac{1}{|z-\tilde{z}|}\,\mathrm{d}z\,\mathrm{d}\tilde{z} + \frac{\rho^2 l^4}{2}\int_{Q_{L/l}}\int_{Q_{L/l}}\ln\frac{1}{|z-\tilde{z}|}\,\mathrm{d}z\,\mathrm{d}\tilde{z}\,.
\end{aligned}$$

By Newton's theorem one has

$$\int_{x+B_R}\int_{y+B_R}\ln\frac{1}{|z-\tilde{z}|}\,\mathrm{d}z\,\mathrm{d}\tilde{z} \;=\; \pi^2R^4\ln\frac{1}{|x-y|}.$$

Furthermore,

$$\begin{aligned}
&-\sum_{x\in\mathcal{C}_{\rho,L}}\rho l^4\int_{x+B_R}\int_{Q_{L/l}}\ln\frac{1}{|z-\tilde z|}\,\mathrm{d}z\,\mathrm{d}\tilde z\\
&=-\sum_{x\in\mathcal{C}_{\rho,L}}\rho l^4\pi R^2\int_{Q_{L/l}\setminus(x+B_R)}\ln\frac{1}{|z-x|}\,\mathrm{d}z-\sum_{x\in\mathcal{C}_{\rho,L}}\rho l^4\int_{x+B_R}\int_{x+B_R}\ln\frac{1}{|z-\tilde z|}\,\mathrm{d}z\,\mathrm{d}\tilde z\\
&=-\rho^2 l^4\sum_{x\in\mathcal{C}_{\rho,L}}\int_{Q_{L/l}}\ln\frac{1}{|z-x|}\,\mathrm{d}z+\rho^2 l^4\sum_{x\in\mathcal{C}_{\rho,L}}\int_{x+B_R}\ln\frac{1}{|z-x|}\,\mathrm{d}z\\
&\quad-\rho l^4 N\pi^2R^4\Big(\ln\frac{1}{R}+\frac14\Big)\\
&=-\rho^2 l^4\sum_{x\in\mathcal{C}_{\rho,L}}\int_{Q_{L/l}}\ln\frac{1}{|z-x|}\,\mathrm{d}z+\rho^2 l^4N\pi R^2\Big(\ln\frac{1}{R}+\frac12\Big)-\rho l^4 N\pi^2R^4\Big(\ln\frac{1}{R}+\frac14\Big)\\
&=-\rho^2 l^4\sum_{x\in\mathcal{C}_{\rho,L}}\int_{Q_{L/l}}\ln\frac{1}{|z-x|}\,\mathrm{d}z+\frac14\rho^3 l^4N.
\end{aligned}$$

Therefore, with e_{Jellium} as defined above,

$$\begin{aligned}
\mathcal{E}_{\rho,L}(\Omega_{\rho,L})&=|\Omega_{\rho,L}|\Bigg(2\Big(\frac{\pi}{\rho}\Big)^{1/2}\frac1l+\frac{l^2}{4}\rho\Big(\ln\frac{\pi}{\rho}+\frac12\Big)+\rho l^2\frac{l^2}{L^2}\Bigg[\frac12\sum_{x,y\in\mathcal{C}_{\rho,L},x\neq y}\ln\frac{1}{|x-y|}\\
&\qquad-\sum_{x\in\mathcal{C}_{\rho,L}}\int_{Q_{L/l}}\ln\frac{1}{|x_i-z|}\,\mathrm{d}z+\frac12\int_{Q_{L/l}}\int_{Q_{L/l}}\ln\frac{1}{|z-\tilde z|}\,\mathrm{d}z\,\mathrm{d}\tilde z\Bigg]+\frac14\rho^2l^2\Bigg)\\
&=|\Omega_{\rho,L}|\Bigg(2\Big(\frac{\pi}{\rho}\Big)^{1/2}\frac1l+\frac{l^2}{4}\rho\Big(\ln\frac{\pi}{\rho}+\frac12\Big)+\rho l^2 e_{\text{Jellium}}+\frac14\rho^2l^2\Bigg)\\
&\qquad+|\Omega_{\rho,L}|\rho l^2R_{L/l}.
\end{aligned}$$

Here, the error term is defined

$$\begin{aligned}
R_{L/l}:=\frac{l^2}{L^2}\Bigg[&\frac12\sum_{x,y\in\mathcal{C}_{\rho,L},x\neq y}\ln\frac{1}{|x-y|}-\sum_{x\in\mathcal{C}_{\rho,L}}\int_{Q_{L/l}}\ln\frac{1}{|x_i-z|}\,\mathrm{d}z\\
&+\frac12\int_{Q_{L/l}}\int_{Q_{L/l}}\ln\frac{1}{|z-\tilde z|}\,\mathrm{d}z\,\mathrm{d}\tilde z\Bigg]-e_{\text{Jellium}},
\end{aligned}$$

which vanishes as $L\to\infty$ if $\mathcal{C}_{\rho,L}$ is chosen to be a minimizer of jellium.

Note that points of a minimizer $x_1,\dots,x_N\in Q_L$ of jellium are separated by a constant, i.e. $\min_{i\neq j}|x_i-x_j|\geq\delta$ for some universal $\delta>0$ [33, Lemma 25]. The separation that is assumed in the definition of $\mathcal{C}_{\rho,L}$ is arbitrary small since $2R=\frac{2}{\pi^{1/2}}\rho^{1/2}$.

Minimizing $2\big(\frac{\pi}{\rho}\big)^{1/2}\frac1l+l^2A(\rho)$ with respect to $l>0$ yields

$$l:=\Big(\frac{\pi}{\rho}\Big)^{1/6}\frac{1}{A(\rho)^{1/3}},$$

where $A(\rho) := \frac{1}{4}\rho\Big(\ln\frac{\pi}{\rho} + \frac{1}{2}\Big) + \rho e_{\text{Jellium}} + \frac{1}{4}\rho^2$.

Therefore,

$$\begin{aligned}\frac{\mathcal{E}_{\rho,L}(\Omega_{\rho,L})}{|\Omega_{\rho,L}|} &= 3\bigg(\frac{\pi}{\rho}A(\rho)\bigg)^{1/3} + R_{L/l}\\ &= 3\bigg(\frac{\pi}{4}\ln\frac{1}{\rho} + \frac{\pi}{4}\Big(\ln\pi + \frac{1}{2}\Big) + \pi\, e_{\text{Jellium}} + \frac{\pi\rho}{4}\bigg)^{1/3} + R_{L/l}.\end{aligned}$$

This concludes the proof of Proposition 3.4.

□

3.1.2 Lower Bound on the Ground State Energy

In this section, the proof of the lower bound from Theorem 3.1 is given. For convenience this result is restated.

Proposition 3.5 (Lower bound)**.** *There is a constant $C > 0$ such that for all $\rho \in (0, \frac{1}{C}]$, $L > 0$,*

$$\frac{E_{\rho,L}}{\rho L^2} \geq 3\bigg(\frac{\pi}{4}\ln\frac{1}{\rho}\bigg)^{1/3} - \frac{C}{(\ln\frac{1}{\rho})^{2/3}}. \tag{3.8}$$

First of all, replace the logarithmic interaction by the more regular potential

$$Y_\omega(x) = K_0(\omega|x|), \qquad \text{for} \quad x \in \mathbb{R}^2 \quad \text{and} \quad \omega := C_\omega \rho^{1/2}\bigg(\ln\frac{1}{\rho}\bigg)^{1/3}.$$

Here, K_0 denotes the modified Bessel function of second kind of order 0.

Lemma 3.6 (Lower bound on the interaction part)**.** *For all $L > 0$, $\rho \in (0,1)$, $\omega > 0$ and for all $\Omega_{\rho,L} \subset Q_L$ with $|\Omega_{\rho,L}| = \rho L^2$, one has*

$$\begin{aligned}&\frac{1}{2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}\Big(1_{\Omega_{\rho,L}}(x) - \rho 1_{Q_L}(x)\Big)\ln\frac{1}{|x-y|}\Big(1_{\Omega_{\rho,L}}(y) - \rho 1_{Q_L}(y)\Big)\,\mathrm{d}x\,\mathrm{d}y\\ &\geq \frac{1}{2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} 1_{\Omega_{\rho,L}}(x)\, Y_\omega(x-y)\, 1_{\Omega_{\rho,L}}(y)\,\mathrm{d}x\,\mathrm{d}y - 2\pi\rho|\Omega_{\rho,L}|\omega^{-2}.\end{aligned}$$

Proof. The following estimate holds for the Fourier transform.

$$\mathfrak{F}[-\ln|\cdot|](k) = \frac{1}{|k|^2} \geq \frac{1}{|k|^2 + \omega^2} = \mathfrak{F}[Y_\omega](k).$$

Here, the convention is used $\mathfrak{F}[f](k) := \frac{1}{2\pi}\int_{\mathbb{R}^2} f(x)e^{-ikx}\,\mathrm{d}x$ for $f \in L^1(\mathbb{R}^2)$. Note that neutrality ensures $\mathfrak{F}[1_{\Omega_{\rho,L}} - \rho 1_{Q_L}](0) = 0$. Furthermore, $\mathfrak{F}[1_{\Omega_{\rho,L}} - \rho 1_{Q_L}] \in C^1(\mathbb{R}^2)$ because

$1_{\Omega_{\rho,L}} - \rho 1_{Q_L}$ has bounded support. Thus, $\mathfrak{F}[1_{\Omega_{\rho,L}} - \rho 1_{Q_L}]/|k|^2$ is integrable at 0. Therefore,

$$\begin{aligned}&\frac{1}{2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}\Big(1_{\Omega_{\rho,L}}(x) - \rho 1_{Q_L}(x)\Big)\ln\frac{1}{|x-y|}\Big(1_{\Omega_{\rho,L}}(y) - \rho 1_{Q_L}(y)\Big)\,\mathrm{d}x\,\mathrm{d}y\\ \geq &\frac{1}{2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}\Big(1_{\Omega_{\rho,L}}(x) - \rho 1_{Q_L}(x)\Big)Y_\omega(x-y)\Big(1_{\Omega_{\rho,L}}(y) - \rho 1_{Q_L}(y)\Big)\,\mathrm{d}x\,\mathrm{d}y\,.\end{aligned}$$

One arrives at the estimate stated in the lemma through the simple calculation

$$\begin{aligned}&\frac{1}{2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}\Big(1_{\Omega_{\rho,L}}(x) - \rho 1_{Q_L}(x)\Big)Y_\omega(x-y)\Big(1_{\Omega_{\rho,L}}(y) - \rho 1_{Q_L}(y)\Big)\,\mathrm{d}x\,\mathrm{d}y\\ \geq &\frac{1}{2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}1_{\Omega_{\rho,L}}(x)Y_\omega(x-y)1_{\Omega_{\rho,L}}(y)\,\mathrm{d}x\,\mathrm{d}y - \rho\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}1_{\Omega_{\rho,L}}(x)Y_\omega(x-y)1_{Q_L}(y)\,\mathrm{d}x\,\mathrm{d}y\\ \geq &\frac{1}{2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}1_{\Omega_{\rho,L}}(x)Y_\omega(x-y)1_{\Omega_{\rho,L}}(y)\,\mathrm{d}x\,\mathrm{d}y - 2\pi\rho|\Omega_{\rho,L}|\omega^{-2}.\end{aligned}$$

Here, the fact is used that $\int_0^\infty K_0(r)r\,\mathrm{d}r = 1$. □

For $\Omega_{\rho,L} \subset Q_L$ with $|\Omega_{\rho,L}| = \rho L^2$, let $J \subset \mathbb{N}$ and

$$\Omega_{\rho,L} = \bigcup_{j\in J}\Omega_j \qquad \text{with connected } \Omega_j \text{ and } \Omega_i \cap \Omega_j = \emptyset \text{ for } i \neq j.$$

To prove Proposition 3.5 neglect the interaction of different connected components. By Lemma 3.6, one has

$$\begin{aligned}\mathcal{E}_{\rho,L}(\Omega_{\rho,L}) &\geq \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}1_{\Omega_{\rho,L}}(x)\,Y_\omega(x-y)\,1_{\Omega_{\rho,L}}(y)\,\mathrm{d}x\,\mathrm{d}y - 2\pi\rho|\Omega_{\rho,L}|\omega^{-2}\\ &\geq \sum_{j\in J}\left(\mathrm{Per}(\Omega_j) + \frac{1}{2}\int_{\Omega_j}\int_{\Omega_j}K_0(\omega|x-y|)\,\mathrm{d}x\,\mathrm{d}y\right) - 2\pi\rho|\Omega_{\rho,L}|\omega^{-2}.\end{aligned} \tag{3.9}$$

Now, distinguish different cases depending on $\mathrm{diam}(\Omega_j)$.

Case 1: Suppose $\mathrm{diam}(\Omega_j) \leq \frac{C_1}{(\ln\frac{1}{\rho})^{1/3}}$. Then,

$$\begin{aligned}&\mathrm{Per}(\Omega_j) + \frac{1}{2}\int_{\Omega_j}\int_{\Omega_j}K_0(\omega|x-y|)\,\mathrm{d}x\,\mathrm{d}y\\ &\geq \mathrm{Per}(\Omega_j) + \frac{1}{2}|\Omega_j|^2 K_0(\omega\,\mathrm{diam}(\Omega_j))\\ &\geq \sqrt{4\pi|\Omega_j|} + \frac{1}{2}|\Omega_j|^2\ln\left(\frac{1}{C_1 C_\omega\rho^{1/2}}\right)\\ &\geq |\Omega_j|\inf_{t>0}\left(\frac{\sqrt{4\pi}}{t} + \frac{t^2}{2}\ln\left(\frac{1}{C_1 C_\omega\rho^{1/2}}\right)\right)\\ &\geq 3\left(\frac{\pi}{4}\ln\frac{1}{\rho}\right)^{1/3}|\Omega_j| - \frac{C|\Omega_j|}{(\ln\frac{1}{\rho})^{2/3}},\end{aligned}$$

if $C > 2\left(\frac{\pi}{4}\right)^{1/3}\ln(C_1 C_\omega)$. Here, the isoperimetric inequality $\mathrm{Per}(\Omega^{(m)}) \geq 2\pi^{1/2}|\Omega^{(m)}|^{1/2}$ is used and the inequality $K_0(r) \geq \ln\frac{1}{r}$ for $r > 0$.

Case 2: Suppose $\mathrm{diam}(\Omega_j) > \frac{C_1}{(\ln\frac{1}{\rho})^{1/3}}$ and $|\Omega_j|^{1/2} \leq \frac{C_2}{(\ln\frac{1}{\rho})^{1/3}}$. Then, $1 \geq \frac{|\Omega_j|^{1/2}(\ln\frac{1}{\rho})^{1/3}}{C_2}$ and thus,

$$\begin{aligned}\mathrm{Per}(\Omega_j) &\geq \mathrm{diam}(\Omega_j)\\ &> \frac{C_1}{(\ln\frac{1}{\rho})^{1/3}}\\ &\geq \frac{C_1}{C_2^2}|\Omega_j|\left(\ln\frac{1}{\rho}\right)^{1/3}.\end{aligned}$$

This is the desired inequality, if $\frac{C_1}{C_2^2} \geq 3\left(\frac{\pi}{4}\right)^{1/3}$.

Case 3: Suppose $\frac{C_1}{(\ln\frac{1}{\rho})^{1/3}} < \mathrm{diam}\,\Omega_j \leq C_3\left(\ln\frac{1}{\rho}\right)^{2/3}$ and $|\Omega_j|^{1/2} > \frac{C_2}{(\ln\frac{1}{\rho})^{1/3}}$. Then,

$$\begin{aligned}\frac{1}{2}\int_{\Omega_j}\int_{\Omega_j} K_0(\omega|x-y|)\,\mathrm{d}x\,\mathrm{d}y &\geq \frac{1}{2}|\Omega_j|^2 K_0(\omega\,\mathrm{diam}(\Omega_j))\\ &\geq \frac{1}{2}|\Omega_j|^2\ln\left(\frac{1}{C_3 C_\omega \rho^{1/2}\ln\frac{1}{\rho}}\right)\\ &\geq \frac{1}{8}|\Omega_j|^2\ln\frac{1}{\rho}\\ &\geq \frac{C_2^2}{8}|\Omega_j|\left(\ln\frac{1}{\rho}\right)^{1/3},\end{aligned}$$

if ρ is sufficiently small. This is the desired inequality, if $\frac{C_2^2}{8} \geq 3\left(\frac{\pi}{4}\right)^{1/3}$.

Case 4: Suppose $\mathrm{diam}\,\Omega_j > C_3\left(\ln\frac{1}{\rho}\right)^{2/3}$ and $|\Omega_j|^{1/2} > \frac{C_2}{(\ln\frac{1}{\rho})^{1/3}}$.
Solve this case by localizing the problem to smaller boxes. The following lemma is useful to control the behavior of the perimeter term under this localization.

Lemma 3.7 (Localization of the perimeter term)**.** *Let $\Omega \subset \mathbb{R}^2$ have finite perimeter. Then, for every $R > 0$,*

$$\mathrm{Per}(\Omega) \geq \sum_{m\in\mathbb{Z}^2}\int_{Q_1}\mathrm{Per}(\Omega\cap Q_R(m+\mu))\,\mathrm{d}\mu - \frac{4|\Omega|}{R}.$$

Proof. In every box, the boundary of $\Omega \cap Q_R(m+\mu)$ consists of two parts: the portion of $\partial\Omega$ lying inside $Q_R(m+\mu)$, and the portion of Ω intersecting $\partial Q_R(m+\mu)$, which is added by partitioning Ω into boxes. One therefore has that

$$\begin{aligned}
&\sum_{m\in\mathbb{Z}^2}\int_{Q_1}\mathrm{Per}(\Omega\cap Q_R(m+\mu))\,\mathrm{d}\mu\\
&\le \int_{Q_1}\sum_{m\in\mathbb{Z}^2}\mathcal{H}^1(\partial\Omega\cap Q_R(m+\mu))\,\mathrm{d}\mu+\int_{Q_1}\sum_{m\in\mathbb{Z}^2}\mathcal{H}^1(\Omega\cap\partial Q_R(m+\mu))\,\mathrm{d}\mu\\
&\le \mathrm{Per}(\Omega)+\int_{Q_1}\sum_{m\in\mathbb{Z}^2}\mathcal{H}^1(\Omega\cap\partial Q_R(m+\mu))\,\mathrm{d}\mu\,. \qquad (3.10)
\end{aligned}$$

It remains to evaluate the second term in (3.10). Since all sets appearing there are subsets of the boundaries of squares, decompose

$$\bigcup_{m\in\mathbb{Z}^2}\Omega\cap\partial Q_R(m+\mu)=\bigcup_{i=1}^{2}\bigcup_{l\in\mathbb{Z}}\Omega\cap\Big\{x\in\mathbb{R}^2:\ x_i=R\Big(l+\frac{1}{2}+\mu_i\Big)\Big\},$$

i.e. 'slices' of $\Omega\cap\partial Q_R(m+\mu)$ are distinguished according to the coordinate axis they are parallel to. Note that $\mathcal{H}^1$- almost every point in one axis is contained in the boundary of exactly two squares adjacent to the axis. Since the union $\bigcup_{i=1}^2$ is disjoint up to an $\mathcal{H}^1$-null set, one therefore obtains

$$\int_{Q_1}\sum_{m\in\mathbb{Z}^2}\mathcal{H}^1(\Omega\cap\partial Q_R(m+\mu))\,\mathrm{d}\mu=2\sum_{i=1}^{2}\int_{[-1/2,1/2]^2}\sum_{l\in\mathbb{Z}}\mathcal{H}^1(\Omega\cap\{x_i=R(l+1/2+\mu_i)\})\,\mathrm{d}\mu_1\,\mathrm{d}\mu_2\,.$$

Note that the integrand on the right hand side only depends on *one* of the μ_i. One can therefore do the $\mathrm{d}\mu_j$-integration with $j\neq i$ to find that

$$\begin{aligned}
&\int_{Q_1}\sum_{m\in\mathbb{Z}^2}\mathcal{H}^1(\Omega\cap\partial Q_R(m+\mu))\,\mathrm{d}\mu=2\sum_{i=1}^{2}\int_{-1/2}^{1/2}\sum_{l\in\mathbb{Z}}\mathcal{H}^1(\Omega\cap\{x_i=R(l+1/2+\mu_i)\})\,\mathrm{d}\mu_i\\
&=2\sum_{i=1}^{2}\int_{\mathbb{R}}\mathcal{H}^1(\Omega\cap\{x_i=R\mu_i\})\,\mathrm{d}\mu_i=\frac{2}{R}\sum_{i=1}^{2}\int_{\mathbb{R}}\mathcal{H}^1(\Omega\cap\{x_i=\mu_i\})\,\mathrm{d}\mu_i=\frac{4|\Omega|}{R}
\end{aligned}$$

by Fubini's theorem. Plugging this in (3.10) completes the proof of Lemma 3.7. □

Let $R:=\frac{C_3}{\sqrt{2}}\Big(\ln\frac{1}{\rho}\Big)^{2/3}$. Ω_j is the (finite) disjoint union

$$\Omega_j=\bigcup_{m\in\mathbb{Z}^2}\Big(\Omega_j\cap Q_R(m+\mu_j)\Big)=:\bigcup_{m\in\mathbb{Z}^2}\Omega_j^{(m)} \qquad (3.11)$$

for some $\mu_j\in Q_1$ to be chosen below. Note that the choice of $\Omega_j^{(m)}$ in (3.11) ensures that $\mathrm{diam}(\Omega_j^{(m)})\le\sqrt{2}R=C_3\Big(\ln\frac{1}{\rho}\Big)^{2/3}$.

Then, one can estimate the energy from below as follows.

$$\begin{aligned}
&\mathrm{Per}(\Omega_j)+\frac{1}{2}\int_{\Omega_j}\int_{\Omega_j}K_0(\omega|x-y|)\,\mathrm{d}x\,\mathrm{d}y\\
&\ge\sum_{m\in\mathbb{Z}^2}\Big(\mathrm{Per}(\Omega^{(m)})+\frac{1}{2}\int_{\Omega_j^{(m)}}\int_{\Omega_j^{(m)}}K_0(\omega|x-y|)\,\mathrm{d}x\,\mathrm{d}y\Big)+\mathcal{P} \qquad (3.12)
\end{aligned}$$

with the perimeter error term $\mathcal{P} := \mathrm{Per}(\Omega) - \sum_{m\in\mathbb{Z}} \mathrm{Per}(\Omega^{(m)})$. Since $\mathrm{diam}(\Omega_j^{(m)}) \leq C_3\Big(\ln \frac{1}{\rho}\Big)^{2/3}$, one can apply cases 1-3 to get the desired lower bound.

It remains to bound the perimeter error $\mathcal{P}$ appropriately. By Lemma 3.7 the averaged estimate holds

$$\int_{Q_1} \left(\sum_{m\in\mathbb{Z}^2} \mathrm{Per}(\Omega_j \cap Q_R(m+\mu)) \right) \mathrm{d}\mu \leq \mathrm{Per}(\Omega_j) + \frac{4|\Omega_j|}{R}, \tag{3.13}$$

and therefore there exists $\mu_j \in Q_1$ depending on Ω_j such that

$$\sum_{m\in\mathbb{Z}^2} \mathrm{Per}(\Omega_j \cap Q_R(m+\mu_j)) \leq \mathrm{Per}(\Omega_j) + \frac{4|\Omega_j|}{R}. \tag{3.14}$$

With this choice of μ_j, one arrives at the bound

$$\mathcal{P} = \mathrm{Per}(\Omega_j) - \sum_{m\in\mathbb{Z}} \mathrm{Per}(\Omega_j^{(m)}) \geq -\frac{4|\Omega_j|}{R} = -\frac{4\sqrt{2}}{C_3\Big(\ln\frac{1}{\rho}\Big)^{2/3}}|\Omega_j| \tag{3.15}$$

This concludes the proof of Proposition 3.5.

3.1.3 Concerning the mass and shape of the droplets

Consider a minimizer $\Omega_{\rho,L}$ of $\mathcal{E}_{\rho,L}$ over all $\Omega_{\rho,L} \subset Q_L$ such that one has charge neutrality $|\Omega_{\rho,L}| = \rho L^2$. Let $\Omega_{\rho,L} = \bigcup_{j\in J} \Omega_j$ with $\Omega_{j_1} \cap \Omega_{j_2} = \emptyset$ for $j_1 \neq j_2$ and connected Ω_j for all $j \in J$. By Lemma 3.7 one may assume $\mathrm{diam}(\Omega_j) \leq C(\ln\frac{1}{\rho})^{2/3}$ for all $j \in J$ and

$$\mathrm{Per}(\Omega_{\rho,L}) \geq \sum_{j\in J} \mathrm{Per}(\Omega_j) - \frac{C|\Omega_{\rho,L}|}{(\ln\frac{1}{\rho})^{2/3}}.$$

In this section Corollary 3.2 is proven. The argument is similar to what is done in [25]. By Proposition 3.4 it is known

$$\begin{aligned}
&3\left(\frac{\pi}{4}\ln\frac{1}{\rho}\right)^{1/3}\rho L^2 + \frac{C\rho L^2}{(\ln\frac{1}{\rho})^{2/3}} \geq \mathcal{E}_{\rho,L}(\Omega_{\rho,L}) \\
&= \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L}\int_{Q_L} (1_{\Omega_{\rho,L}}(x) - \rho) \ln\frac{1}{|x-y|}(1_{\Omega_{\rho,L}}(y) - \rho)\,\mathrm{d}x\,\mathrm{d}y \\
&\geq \mathrm{Per}(\Omega_{\rho,L}) + \frac{1}{2}\int_{Q_L}\int_{Q_L} (1_{\Omega_{\rho,L}}(x) - \rho) K_0(\omega|x-y|)(1_{\Omega_{\rho,L}}(y) - \rho)\,\mathrm{d}x\,\mathrm{d}y \\
&\geq \sum_{j\in J}\left(\mathrm{Per}(\Omega_j) + \frac{1}{2}\int_{\Omega_j}\int_{\Omega_j} \ln\frac{1}{\omega|x-y|}\,\mathrm{d}x\,\mathrm{d}y \right) - \frac{C\rho L^2}{(\ln\frac{1}{\rho})^{2/3}}.
\end{aligned}$$

Here, K_0 is the modified Bessel function of second kind of order 0 and $\omega := C_\omega \rho^{1/2}(\ln\frac{1}{\rho})^{1/3}$. In the last inequality the fact is used that $K_0(r) \geq \ln\frac{1}{r}$ for $r > 0$.

Define $J_0 := \{j \in J : \mathrm{diam}(\Omega_j) \le C_1(\ln \frac{1}{\rho})^{-1/3}\}$. In the proof of the lower bound the self-energy of droplets Ω_j with $j \in J_0$ is estimated from below by minimizing over all masses. Now, one can get a result about the mass and shape of the droplets by expanding the energy about this optimal mass $\kappa := \frac{2^{4/3}\pi^{1/3}}{(\ln \frac{1}{\rho})^{2/3}}$. For $j \in J_0$, one has

$$\sqrt{4\pi|\Omega_j|} + \frac{1}{2}\int_{\Omega_j}\int_{\Omega_j} \ln \frac{1}{\omega|x-y|}\,\mathrm{d}x\,\mathrm{d}y$$
$$\ge 3\left(\frac{\pi}{4}\ln\frac{1}{\rho}\right)^{1/3}|\Omega_j| + \frac{3\pi^{1/3}}{2^{8/3}}\left(\ln\frac{1}{\rho}\right)^{1/3}|\Omega_j|\left(\frac{|\Omega_j|}{\kappa}-1\right)^2 - \frac{C|\Omega_j|}{(\ln\frac{1}{\rho})^{2/3}}.$$

For $j \in J\backslash J_0$ the proof of the lower bound implies

$$\mathrm{Per}(\Omega_j) + \frac{1}{2}\int_{\Omega_j}\int_{\Omega_j} \ln\frac{1}{\omega|x-y|}\,\mathrm{d}x\,\mathrm{d}y \ge C\left(\ln\frac{1}{\rho}\right)^{1/3} - \frac{C|\Omega_j|}{(\ln\frac{1}{\rho})^{2/3}},$$

with $C > 3(\frac{\pi}{4})^{1/3}$.

These estimates imply the following bound

$$\frac{C\rho L^2}{(\ln\frac{1}{\rho})^{2/3}} \ge \mathcal{E}_{\rho,L}(\Omega_{\rho,L}) - 3\left(\frac{\pi}{4}\ln\frac{1}{\rho}\right)^{1/3}\rho L^2$$
$$\ge \sum_{j\in J_0}\left(\mathrm{Per}(\Omega_j) - \sqrt{4\pi|\Omega_j|}\right) + \sum_{j\in J_0}\frac{3\pi^{1/3}}{2^{8/3}}\left(\ln\frac{1}{\rho}\right)^{1/3}|\Omega_j|\left(\frac{|\Omega_j|}{\kappa}-1\right)^2$$
$$+\sum_{j\in J\backslash J_0}\left(C - 3\left(\frac{\pi}{4}\right)^{1/3}\right)\left(\ln\frac{1}{\rho}\right)^{1/3}|\Omega_j| - \frac{C\rho L^2}{(\ln\frac{1}{\rho})^{2/3}},$$

with $C > 3(\frac{\pi}{4})^{1/3}$.

Define

$$J_\epsilon := \left\{ j \in J : \frac{\mathrm{Per}(\Omega_j)}{\sqrt{4\pi|\Omega_j|}} - 1 > \epsilon \quad \text{or} \quad \left(\frac{|\Omega_j|}{\kappa}-1\right)^2 > \epsilon \right\}.$$

If $(\frac{|\Omega_j|}{\kappa}-1)^2 \le \epsilon \le \frac{1}{4}$, then $\sqrt{4\pi|\Omega_j|} \ge \frac{1}{C}|\Omega_j|(\ln\frac{1}{\rho})^{1/3}$. Therefore, one has

$$\frac{C\rho L^2}{(\ln\frac{1}{\rho})^{2/3}} \ge \sum_{j\in J_0\cap J_\epsilon}\frac{1}{C}|\Omega_j|\left(\ln\frac{1}{\rho}\right)^{1/3}\epsilon + \sum_{j\in J\backslash J_0} C\left(\ln\frac{1}{\rho}\right)^{1/3}|\Omega_j|$$
$$\ge \sum_{j\in J_\epsilon}\frac{1}{C}|\Omega_j|\left(\ln\frac{1}{\rho}\right)^{1/3}\epsilon = \frac{m_\epsilon}{C}\left(\ln\frac{1}{\rho}\right)^{1/3}\epsilon.$$

This is equivalent to the corollary

$$\frac{m_\epsilon}{|\Omega_{\rho,L}|} \le \frac{C}{\epsilon\ln\frac{1}{\rho}}.$$

So the relative mass of all droplets which are not close to the optimal mass κ or not close to the optimal shape (that is a disk), tends to zero as ρ tends to zero.

3.2 Uniform Distribution of Energy for Minimizers

In this section, it is proven that the energy of a minimizer of the liquid drop model with Neumann boundary condition in a cube $Q_L := (-L/2, L/2)^d$ with $d \geq 2$ is uniformly distributed on a smaller scale $R \leq L$. The proof is similar to the proof of Theorem 4 in [2].

Let $\Omega \subset \mathbb{R}^d$, $Q \subseteq \mathbb{R}^d$ and $\mathbf{b} \in L^2(Q, \mathbb{R}^d)$. As in [1], define

$$\mathcal{E}(\Omega, \mathbf{b}, Q) := \operatorname{Per}(\Omega \cap Q) + \frac{1}{2} \int_Q |\mathbf{b}|^2 \, \mathrm{d}x$$

and the set of admissible $(\Omega, \mathbf{b})$ satisfying Neumann boundary condition

$$\begin{aligned} \mathcal{A}_{\text{Neu}}(\rho, Q) := \Big\{ &(\Omega, \mathbf{b}) \mid \Omega \subset Q \text{ and } \mathbf{b} \in L^2(Q, \mathbb{R}^d) \text{ with } |\Omega| = \rho |Q| \text{ such that} \\ &\nabla \mathbf{b} = 1_\Omega - \rho \text{ in } Q \text{ and } \mathbf{b} \cdot \nu = 0 \text{ on } \partial Q \Big\}. \end{aligned}$$

Furthermore, define the minimal energy

$$E_{\text{Neu}}(\rho, Q) := \inf \{ \mathcal{E}(\Omega, \mathbf{b}, Q) : \ (\Omega, \mathbf{b}) \in \mathcal{A}_{\text{Neu}}(\rho, Q) \}.$$

Let $c_{2,\rho} := (\ln \frac{1}{\rho})^{1/3}$ and $c_{d,\rho} = 1$ for $d \geq 3$. The main result of this section is the following theorem which is formulated for dimensions $d \in \mathbb{N}$, $d \geq 2$.

Theorem 3.8 (Uniform distribution of energy)**.** *Let $(\Omega_{\rho,L}, \mathbf{b}_{\rho,L})$ be a minimizer of $\mathcal{E}(\cdot, \cdot, Q_L)$ over $\mathcal{A}_{\text{Neu}}(\rho, Q_L)$. If $\rho \in (0, \frac{1}{2}]$ and $L \geq R > C c_{d,\rho}^{1/2} \rho^{-1/2}$, then for all $a \in Q_L$ such that $Q_R(a) \subseteq Q_L$ the following upper bound for the local energy holds*

$$\begin{aligned} \mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a)) \leq{} & E_{\text{Neu}}(\rho, Q_R(a)) + C c_{d,\rho}^{(d+2)/(d+1)} \rho^{d/(d+1)} R^{d-2/(d+1)} \\ & + 2\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_R(a) \backslash \partial Q_L) \end{aligned} \tag{3.16}$$

and the lower bound

$$\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a)) \geq E_{\text{Neu}}(\rho, Q_R(a)) - C c_{d,\rho}^{(d+2)/(d+1)} \rho^{d/(d+1)} R^{d-2/(d+1)}. \tag{3.17}$$

Remark 3.9. If $R \geq C \delta^{-(d+1)/2} c_{d,\rho}^{1/2} \rho^{-1/2}$, the first error term in equation (3.16) can be estimated as

$$C c_{d,\rho}^{(d+2)/(d+1)} \rho^{d/(d+1)} R^{d-2/(d+1)} \leq \delta c_{d,\rho} \rho R^d.$$

Remark 3.10. The boundary term in equation (3.16) can be crudely estimated $\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_R(a)) \leq C R^{d-1}$. However, for minimizers $\Omega_{\rho,L}$ local neutrality is expected, that is $|\Omega_{\rho,L} \cap Q_R(a)| \approx \rho R^d$. In this case, averaging over boundaries gives the better bound $2\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_R(a)) \leq C \rho R^{d-1}$.

Remark 3.11. The error term in this formulation of uniform distribution of energy is a decent estimate for scales R that are close to the minimal length scale $Cc_{d,\rho}^{1/2}\rho^{-1/2}$. In the dilute limit that is considered in this thesis ρ is very small. This is why, the factor $\rho^{d/(d+1)}$ is more important than having an error term proportional to R^{d-1}. However, if one is interested in large length scales $R > Cc_{d,\rho}^{1/2}\rho^{-1}$, it is more important to have an error term proportional to R^{d-1}. With the method of Armstrong and Serfaty [2] it is also possible to prove uniform distribution of energy of the form

$$\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a)) = E_{\text{Neu}}(\rho, Q_R(a)) + \mathcal{O}(R^{d-1}), \tag{3.18}$$

for R sufficiently large. Here, the error $\mathcal{O}(R^{d-1})$ might depend on $\rho > 0$.

To prove uniform distribution of energy a simple estimate on the minimal Neumann energy is needed.

Lemma 3.12 (Simple energy estimate)**.** *Let $U = \bigcup_{i\in I} U_i$ be the disjoint union of cuboids U_i with side lengths in $[\frac{1}{2}l, l]$ where $l \geq Cc_{d,\rho}^{-1}\rho^{-1/d}$ and $\rho \in (0, \frac{1}{2})$. I.e. for $i \in I$ assume there exists $\boldsymbol{l}^{(i)} \in [\frac{1}{2}l, l]^d$ and $r^{(i)} \in U$ such that $U_i = Q_{\boldsymbol{l}^{(i)}}(r^{(i)})$ as defined in* (2.30)*. Then,*

$$E_{\text{Neu}}(\rho, U) \leq Cc_{d,\rho}\rho|U|. \tag{3.19}$$

where $c_{2,\rho} := (\ln \frac{1}{\rho})^{1/3}$ and $c_{d,\rho} := 1$ for $d \geq 3$.

Proof. First of all, the problem is reduced to the length scale $Cc_{d,\rho}^{-1}\rho^{-1/d}$. To get a simple upper bound for the Neumann energy, one can then evaluate the energy of a ball.

Since the Neumann energy is sub-additive one has

$$E_{\text{Neu}}(\rho, U) \leq \sum_{i\in I} E_{\text{Neu}}(\rho, U_i). \tag{3.20}$$

For simplicity assume $l = C_l c_{d,\rho}^{-1}\rho^{-1/d}$ with $C_l \geq 1$. (If l is larger than that, one can simple sub-divide the cuboids U_i in smaller ones and relabel them.) Since cuboids of different centers are equivalent it suffices to consider $U_i = Q_{\boldsymbol{l}^{(i)}} =: Q$ for a general $\boldsymbol{l}^{(i)} \in [\frac{1}{2}l, l]^d$. Let $\lambda := |Q|/l^d$ and $R > 0$ be such that the d dimensional ball of radius R centered at 0 which is denoted by B_R has mass $\lambda\rho$, that is $|B_R| = \lambda\rho$. Then, $|lB_R| = \lambda\rho l^d = \rho|Q|$. Let $v \in H^2(Q)$ be the solution with mean zero of the Poisson equation

$$\begin{cases} -\Delta v = 1_{lB_R} - \rho & \text{in } Q, \\ \nu\boldsymbol{\nabla} v = 0 & \text{on } \partial Q, \end{cases} \tag{3.21}$$

where ν is the outer normal of ∂Q. Clearly $(lB_R, \boldsymbol{\nabla} v) \in \mathcal{A}_{\text{Neu}}(\rho, Q)$ and therefore,

$$\begin{aligned} E_{\text{Neu}}(\rho, Q_l) &\leq \mathcal{E}(lB_R, \boldsymbol{\nabla} v, Q) = \text{Per}(lB_R) + \frac{1}{2}\int_Q |\boldsymbol{\nabla} v|^2 \,\mathrm{d}x \\ &= l^{d-1}\,\text{Per}(B_R) + \frac{1}{2}\int_Q (-\Delta v)v \,\mathrm{d}x \\ &= l^{d-1}\,\text{Per}(B_R) + \frac{1}{2c_d}\int_Q\int_Q (1_{lB_R} - \rho)G_{\text{Neu}}(x,y)(1_{lB_R} - \rho)\,\mathrm{d}x\,\mathrm{d}y \\ &= l^{d-1}\,\text{Per}(B_R) + \frac{1}{2c_d}\int_{lB_R}\int_{lB_R} G_{\text{Neu}}(x,y)\,\mathrm{d}x\,\mathrm{d}y\,. \end{aligned}$$

Here, G_{Neu} is the Green function of the Poisson equation on Q with Neumann boundary condition which fulfills $\int_Q G_{\mathrm{Neu}}(x,y)\,\mathrm{d}x = 0$ for $y \in Q$. The coefficient $c_2 = 2\pi$ and $c_d = (d-2)|\mathbb{S}^{d-1}|$ for $d \geq 3$ should not be confused with $c_{d,\rho}$. Since $\operatorname{dist}(lB_R, \partial Q)$ is large, Proposition A1 in [2] states for $y \in lB_R$

$$\sup_{x\in Q}\left|G_{\mathrm{Neu}}(x,y) - G(x-y) + |Q|^{-1}\int_Q G(x-z)\,\mathrm{d}z\right| \leq C. \tag{3.22}$$

As defined in the introduction G denotes the fundamental solution of the Poisson equation. So in two dimensions $G(x) = \ln\frac{1}{|x|}$ for $x \in \mathbb{R}^2$ and in d dimensions with $d \geq 3$ it is $G(x) = \frac{1}{|x|^{d-2}}$ for $x \in \mathbb{R}^d$.

Since $|lB_R| \leq \rho l^d = c_{d,\rho}^{-d} \leq 1$, the Neumann ground state energy can be estimated

$$\begin{aligned}
E_{\mathrm{Neu}}(\rho, U_i) &\leq l^{d-1}\operatorname{Per}(B_R) + \frac{1}{2c_d}\int_{lB_R}\int_{lB_R}\left(G(x-y) - |Q|^{-1}\int_{Q_l} G(x-z)\,\mathrm{d}z + C\right)\mathrm{d}x\,\mathrm{d}y \\
&= l^d\left(\frac{1}{l}\operatorname{Per}(B_R) + \frac{l^2}{2c_d}\int_{B_R}\int_{B_R}\left(G(x-y) - \lambda^{-1}\int_{Q/l} G(x-z)\,\mathrm{d}z\right)\mathrm{d}x\,\mathrm{d}y + Cl^dR^{2d}\right) \\
&\leq Cl^d c_{d,\rho}\rho^{1/d}\rho^{1-1/d} + Cl^d c_{d,\rho}^{-2}\rho^{-2/d}\rho c_{d,\rho}^3 R^2 + C\rho l^d c_{d,\rho}^{-d} \leq Cc_{d,\rho}\rho|U_i|.
\end{aligned}$$

This implies for the energy on the whole cube

$$E_{\mathrm{Neu}}(\rho, U) \leq \sum_{i\in I} Cc_{d,\rho}\rho|U_i| = Cc_{d,\rho}\rho|U|. \tag{3.23}$$

□

Similar to Lemma B.4 in [2], the following lemma is formulated.

Lemma 3.13 (Local neutrality)**.** *Let $(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}) \in \mathcal{A}_{\mathrm{Neu}}(\rho, Q_L)$ and let $U \subset Q_L$ be open. Define*

$$\begin{aligned}
U_{+1} &:= \left\{x \in \mathbb{R}^d : x \in U \text{ or } \operatorname{dist}(x,U) < 1\right\} \\
U_{-1} &:= \left\{x \in \mathbb{R}^d : x \in U \text{ and } \operatorname{dist}(x,U) > 1\right\}
\end{aligned}$$

If $\rho \in (0, 1/C]$, then one has the local neutrality bound

$$||\Omega_{\rho,L} \cap U| - \rho|U|| \leq C\operatorname{Per}(U)^{1/2}\|\mathbf{b}_{\rho,L}\|_{L^2(U_{+1}\setminus U_{-1})} + C\rho\operatorname{Per}(U). \tag{3.24}$$

Proof. Let $\chi \in C^1(\mathbb{R}^d)$ be such that $\chi(x) = 1$ for $x \in U$ and $\chi(x) = 0$ for $x \notin U_{+1}$. Then,

$$\begin{aligned}
|\Omega_{\rho,L} \cap U| - \rho|U| &\leq \int_{\mathbb{R}^d}\chi(x)(1_{\Omega_{\rho,L}}(x) - \rho)\,\mathrm{d}x + C\rho\operatorname{Per}(U) \\
&= \int_{\mathbb{R}^d}\chi(x)\nabla\mathbf{b}_{\rho,L}\,\mathrm{d}x + C\rho\operatorname{Per}(U) = -\int_{\mathbb{R}^d}(\boldsymbol{\nabla}\chi(x))\mathbf{b}_{\rho,L}\,\mathrm{d}x + C\rho\operatorname{Per}(U) \\
&\leq \|\boldsymbol{\nabla}\chi\|_2\|\mathbf{b}_{\rho,L}\|_{L^2(\operatorname{supp}\boldsymbol{\nabla}\chi)} + C\rho\operatorname{Per}(U) \\
&\leq C(\operatorname{Per}(U))^{1/2}\|\mathbf{b}_{\rho,L}\|_{L^2(U_{+1}\setminus U)} + C\rho\operatorname{Per}(U).
\end{aligned}$$

Similarly, let $\phi \in C^1(\mathbb{R}^d)$ be such that $\phi(x) = 1$ for $x \in U_{-1}$ and $\phi(x) = 0$ for $x \notin U$. Then,

$$\begin{aligned}\rho|U| - |\Omega_{\rho,L} \cap U| &\leq \int_{\mathbb{R}^d} \phi(x)(\rho - 1_{\Omega_{\rho,L}}(x))\,\mathrm{d}x + C\rho\,\mathrm{Per}(U)\\ &= -\int_{\mathbb{R}^d} \phi(x)\nabla \mathbf{b}_{\rho,L}\,\mathrm{d}x + C\rho\,\mathrm{Per}(U) = \int_{\mathbb{R}^d} (\boldsymbol{\nabla}\phi(x))\mathbf{b}_{\rho,L}\,\mathrm{d}x + C\rho\,\mathrm{Per}(U)\\ &\leq \|\boldsymbol{\nabla}\phi\|_2 \|\mathbf{b}_{\rho,L}\|_{L^2(\mathrm{supp}\,\boldsymbol{\nabla}\phi)} + C\rho\,\mathrm{Per}(U)\\ &\leq C(\mathrm{Per}(U))^{1/2}\|\mathbf{b}_{\rho,L}\|_{L^2(U\setminus U_{-1})} + C\rho\,\mathrm{Per}(U).\end{aligned}$$

□

3.2.1 Upper Bound on the Local Energy

First of all, the following proposition on the uniform distribution of energy is proven. Then, the error is improved in a corollary to get the theorem stated in the beginning.

Proposition 3.14 (Uniform distribution of energy, upper bound)**.** *Let $(\Omega_{\rho,L}, \mathbf{b}_{\rho,L})$ be a minimizer of $\mathcal{E}(\cdot,\cdot,Q_L)$ over $\mathcal{A}_{\mathrm{Neu}}(\rho, Q_L)$. If $\rho \in (0, \frac{1}{2}]$ and $L \geq R \geq Cc_{d,\rho}^{1/2}\rho^{-1/2}$, then one has for all $a \in Q_L$ such that $Q_R(a) \subseteq Q_L$ the local energy estimate*

$$\begin{aligned}\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a)) \leq E_{\mathrm{Neu}}(\rho, Q_R(a)) + Cc_{d,\rho}^{1+1/(2d+3)}\rho^{1-1/(2d+3)}R^{d-1/(d+3/2)}\\ + 2\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_R(a)\setminus\partial Q_L).\end{aligned} \tag{3.25}$$

Furthermore, the neutrality bound $|\Omega_{\rho,L} \cap Q_R(a)| \leq \rho^{1/2}R^d$ holds.

Remark 3.15. In particular, if $R \geq C\delta^{-(d+3/2)}c_{d,\rho}^{1/2}\rho^{-1/2}$, this implies

$$\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a)) \leq E_{\mathrm{Neu}}(\rho, Q_R(a)) + \delta c_{d,\rho}\rho R^d + 2\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_R(a)\setminus\partial Q_L) \tag{3.26}$$

for any $\delta > 0$.

Corollary 3.16. *If the assumptions of Proposition 3.14 hold, then*

$$\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a)) \leq Cc_{d,\rho}\rho R^d. \tag{3.27}$$

Proof. By Lemma 3.12 the Neumann energy can be estimated $E_{\mathrm{Neu}}(\rho, Q_R(a)) \leq Cc_{d,\rho}\rho R^d$. Furthermore, one can find a good boundary that fulfills $\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_R(a)) \leq C\rho^{1/2}R^{d-1}$ by averaging over boundaries as it is done in the proof of the upper bound. □

Proof of Proposition 3.14. The idea of the proof is to change a minimizer locally in $Q_R(a)$. The resulting state gives an upper bound for the energy of a minimizer globally in Q_L. Subtracting the energy in $Q_L\setminus Q_R(a)$, one gets an upper bound for the local energy in $Q_R(a)$.

By assumption $\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_L) = E_{\text{Neu}}(\rho, Q_L)$ and $|\Omega_{\rho,L}| = \rho L^d$. So, assume there exists $L_0 > 0$ such that the local energy is bounded for all $a \in Q_L$ with $Q_{L_0}(a) \subseteq Q_L$

$$\begin{aligned}\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_{L_0}(a)) \leq E_{\text{Neu}}(\rho, Q_{L_0}(a)) + C_0 c_{d,\rho}^{1+1/(2d+3)} \rho^{1-1/(2d+3)} L_0^{d-1/(d+3/2)} \\ + 2\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_{L_0}(a) \backslash \partial Q_L)\end{aligned} \tag{3.28}$$

and such that the neutrality bound holds

$$|\Omega_{\rho,L} \cap Q_{L_0}(a)| \leq \rho^{1/2} L_0^d. \tag{3.29}$$

It will be proven that equation (3.25) holds for all $R \geq L_0/2$. This will also imply the neutrality bound $|\Omega_{\rho,L} \cap Q_R(a)| \leq \rho^{1/2} R^d$. Since this argument can be iterated the result will follow down to scale $R \geq C c_{d,\rho}^{1/2} \rho^{-1/2}$.

Let $(\Omega_1, \mathbf{b}_1)$ be a minimizer of $\mathcal{E}(\cdot, \cdot, Q_R(a))$ over $\mathcal{A}_{\text{Neu}}(\rho, Q_R(a))$ and $(\Omega_2, \mathbf{b}_2)$ be a minimizer of $\mathcal{E}(\cdot, \cdot, Q_L \backslash Q_R(a))$ over $\mathcal{A}_{\text{Neu}}(\rho, Q_L \backslash Q_R(a))$. Define $\Omega := \Omega_1 \cup \Omega_2$ and

$$\mathbf{b}(x) := \begin{cases} \mathbf{b}_1(x) & \text{if } x \in Q_R(a), \\ \mathbf{b}_2(x) & \text{if } x \in Q_L \backslash Q_R(a). \end{cases}$$

Then, $(\Omega, \mathbf{b}) \in \mathcal{A}_{\text{Neu}}(\rho, Q_L)$ and thus

$$\begin{aligned}E_{\text{Neu}}(\rho, Q_L) &\leq \mathcal{E}(\Omega, \mathbf{b}, Q_L) \leq \mathcal{E}(\Omega_1, \mathbf{b}_1, Q_R(a)) + \mathcal{E}(\Omega_2, \mathbf{b}_2, Q_L \backslash Q_R(a)) \\ &= E_{\text{Neu}}(\rho, Q_R(a)) + E_{\text{Neu}}(\rho, Q_L \backslash Q_R(a)),\end{aligned}$$

i.e. the minimal Neumann energy is sub-additive.

Therefore, one has the inequality for the minimizer $(\Omega_{\rho,L}, \mathbf{b}_{\rho,L})$ in Q_L

$$\begin{aligned}&\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a)) + \mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_L \backslash Q_R(a)) \\ &\leq \mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_L) + 2\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_R(a) \backslash \partial Q_L) \\ &= E_{\text{Neu}}(\rho, Q_L) + 2\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_R(a) \backslash \partial Q_L) \\ &\leq E_{\text{Neu}}(\rho, Q_R(a)) + E_{\text{Neu}}(\rho, Q_L \backslash Q_R(a)) + 2\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_R(a) \backslash \partial Q_L).\end{aligned}$$

It remains to prove

$$E_{\text{Neu}}(\rho, Q_L \backslash Q_R(a)) \leq \mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_L \backslash Q_R(a)) + C_0 c_{d,\rho}^{1+1/(2d+3)} \rho^{1-1/(2d+3)} R^{d-1/(d+3/2)}, \tag{3.30}$$

for all $R \geq L_0/2 \geq C c_{d,\rho}^{1/2} \rho^{-1/2}$.

For this purpose, apply the following lemma. (Compare to the inner case of Proposition 4.1 in [2].)

Lemma 3.17. *Let $R \geq \tilde{l} \geq l \geq C c_{d,\rho}^{-1} \rho^{-1/d}$ and assume*

$$S_{\rho,L} := \int_{Q_{R+2\tilde{l}} \backslash Q_{R+\tilde{l}}} |\mathbf{b}_{\rho,L}|^2 \, \mathrm{d}x < \frac{\rho^2}{2^{2d+3}} l^{d+1} \tilde{l}. \tag{3.31}$$

Then,

$$E_{\mathrm{Neu}}(\rho, Q_L \backslash Q_R(a)) \leq \mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_L \backslash Q_R(a)) + C c_{d,\rho} \rho \tilde{l} R^{d-1} + C \frac{l}{\tilde{l}} S_{\rho,L}, \tag{3.32}$$

where the constant $C > 0$ does not depend on C_0.

To make use of the assumption for this iteration step equation (3.28) has to be bounded from above. By Lemma 3.12 the minimal Neumann energy in $Q_{L_0}(a)$ satisfies $E_{\mathrm{Neu}}(\rho, Q_{L_0}(a)) \leq C c_{d,\rho} \rho L_0^d$ if $L_0 \geq C c_{d,\rho}^{-1} \rho^{-1/d}$. Note that the error term is bounded as well $C_0 c_{d,\rho}^{1+1/(2d+3)} \rho^{1-1/(2d+3)} L_0^{d-1/(d+3/2)} \leq c_{d,\rho} \rho L_0^d$ if $L_0 \geq C c_{d,\rho}^{1/2} \rho^{-1/2}$. To bound the surface term in (3.28) from above, one could use the crude estimate $2\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_{L_0}(a)) \leq C L_0^{d-1} \leq C c_{d,\rho} \rho L_0^d$ if $L_0 \geq c_{d,\rho}^{-1} \rho^{-1}$. However, then the iteration would terminate at this length scale for R. To get down to smaller length scales, apply the neutrality assumption (3.29)

$$\frac{1}{2} \int_{3L_0}^{4L_0} \int_{\partial Q_T(a)} 1_{\Omega_{\rho,L}} \, \mathrm{d}x' \, \mathrm{d}T = \int_{Q_{4L_0}(a) \backslash Q_{3L_0}(a)} 1_{\Omega_{\rho,L}} \, \mathrm{d}x \leq |Q_{4L_0}(a) \cap \Omega_{\rho,L}| \leq 4^d \rho^{1/2} L_0^d.$$

Thus, there exists $T \in (3L_0, 4L_0)$ such that

$$\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_T(a)) = \int_{\partial Q_T(a)} 1_{\Omega_{\rho,L}} \, \mathrm{d}x' \leq 2^{2d+1} \rho^{1/2} L_0^{d-1} \leq \rho L_0^d,$$

if $L_0 \geq 2^{2d+1} \rho^{-1/2}$. Therefore, it can be estimated

$$\begin{aligned} S_{\rho,L} &\leq \int_{Q_T(a)} |\mathbf{b}_{\rho,L}|^2 \, \mathrm{d}x \leq 2\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_T(a)) \\ &\leq C c_{d,\rho} \rho L_0^d + \rho L_0^d \\ &\leq C c_{d,\rho} \rho R^d, \end{aligned} \tag{3.33}$$

if $L_0 \geq C c_{d,\rho}^{1/2} \rho^{-1/2}$. Here, the assumption $L_0 \leq 2R$ is used. Note that this constant $C > 0$ does not depend on C_0. It only depends on the upper bound of Lemma 3.12. Minimizing the right hand side of equation (3.32) with respect to $\tilde{l} > 0$ (after estimating $S_{\rho,L}$) gives $\tilde{l} \propto (lR)^{1/2}$. In order to meet condition (3.31), choose $l := C_l (c_{d,\rho} \rho^{-1})^{1/(d+3/2)} R^{1-2/(d+3/2)}$ and thus, $\tilde{l} := C_{\tilde{l}} (c_{d,\rho} \rho^{-1})^{1/(2d+3)} R^{1-1/(d+3/2)}$ with sufficiently large $C_{\tilde{l}} \geq C_l > 0$.

The condition $R \geq \tilde{l} \geq l$ is fulfilled since $R \geq C c_{d,\rho}^{1/2} \rho^{-1/2}$.

By equation (3.32) one gets

$$E_{\mathrm{Neu}}(\rho, Q_L \backslash Q_R(a)) \leq \mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_L \backslash Q_R(a)) + C c_{d,\rho}^{1+1/(2d+3)} \rho^{1-1/(2d+3)} R^{d-1/(d+3/2)},$$

which is (3.30) if C_0 is chosen large enough in the beginning (depending on the constants of Lemmas 3.12 and 3.17).

By Lemma 3.13 and inequality (3.33), one has

$$\begin{aligned} |\Omega_{\rho,L} \cap Q_R(a)| &\leq \rho R^d + C R^{(d-1)/2} \|\mathbf{b}_{\rho,L}\|_{L^2(Q_{R+1}(a))} + C \rho R^{d-1} \\ &\leq \frac{1}{\sqrt{2}} \rho^{1/2} R^d + C c_{d,\rho}^{1/2} \rho^{1/2} R^{d-1/2} + C \rho R^{d-1} \leq \rho^{1/2} R^d, \end{aligned}$$

if $R \geq Cc_{d,\rho}$. This is the neutrality bound (3.29) that is assumed for this iteration and thus, it concludes the proof of Proposition 3.14. □

Proof of Lemma 3.17. The idea is to modify $\Omega_{\rho,L} \cap (Q_L \backslash Q_R(a))$ close to the boundary in such a way that it satisfies the Neumann boundary condition (just as it is done in the proof of Proposition 4.1 in [2]). For this purpose let $\mathcal{O} := Q_L \backslash \overline{Q_T(a)}$ be the old region that is left unchanged and $\mathcal{N} := Q_T(a) \backslash \overline{Q_R(a)}$ be the new region that is changed. Since

$$\frac{1}{2} \int_{R+\tilde{l}}^{R+2\tilde{l}} \int_{\partial Q_T(a)} |\mathbf{b}_{\rho,L}|^2 \, \mathrm{d}x' \, \mathrm{d}T = S_{\rho,L}$$

there exists a $T \in [R+\tilde{l}, R+2\tilde{l}]$ such that

$$\int_{\partial Q_T(a)} |\mathbf{b}_{\rho,L}|^2 \, \mathrm{d}x' \leq \frac{2}{\tilde{l}} S_{\rho,L}. \tag{3.34}$$

The factor 2 is due to the fact that the distance between $\partial Q_{R+\tilde{l}}$ and $\partial Q_{R+2\tilde{l}}$ is $\frac{\tilde{l}}{2}$. One can partition $\mathcal{N}$ into rectangles $Q_l(i) \cap \mathcal{N}$ for $i \in I := \{k \in l\mathbb{Z}^2 : k \in \mathcal{N}\}$ and assume that the constant $C_l > 0$ is chosen such that $\overline{\mathcal{N}} \subset \sum_{i \in I} Q_l(i)$. Then, let $v \in H^2(Q_l(i) \cap \mathcal{N})$ be the solution of the boundary value problem

$$\begin{cases} -\Delta v_i(x) = m_i & \text{for } x \in Q_l(i) \cap \mathcal{N} \\ \boldsymbol{\nabla} v_i(x) \cdot \nu = g_i & \text{for } x \in \partial(Q_l(i) \cap \mathcal{N}) \end{cases}$$

Here, $g_i(x) := -\mathbf{b}_{\rho,L}(x) \cdot \nu$ for $x \in Q_l(i) \cap \partial Q_T$ and $g_i(x) := 0$ for $x \in \partial(Q_l(i) \cap \mathcal{N}) \backslash \partial Q_T$. The solution to this boundary value problem exists because

$$m_i := -(|Q_l(i) \cap \mathcal{N}|)^{-1} \int_{Q_l(i) \cap \partial Q_T} \mathbf{b}_{\rho,L} \cdot \nu \, \mathrm{d}x' .$$

One can estimate

$$\begin{aligned} |m_i| &\leq 2^d l^{-d} \left| \int_{Q_l(i) \cap \partial Q_T} \mathbf{b}_{\rho,L} \cdot \nu \, \mathrm{d}x' \right| \\ &\leq 2^d l^{-(d+1)/2} \left(\int_{Q_l(i) \cap \partial Q_T} |\mathbf{b}_{\rho,L}|^2 \, \mathrm{d}x' \right)^{1/2} \\ &\leq 2^{d+1/2} l^{-(d+1)/2} \tilde{l}^{-1/2} S_{\rho,L}^{1/2} \\ &\leq \frac{\rho}{2}, \end{aligned}$$

where $S_{\rho,L}$ is estimated according to (3.31). Further, let $u_i \in H^2(Q_l(i) \cap \mathcal{N})$ be the solution of the boundary value problem

$$\begin{cases} -\Delta u_i(x) = \sum_{j \in J} 1_{x_j + B_{r_j}}(x) - \rho_i & \text{for } x \in Q_l(i) \cap \mathcal{N}, \\ \boldsymbol{\nabla} u_i(x) \cdot \nu = 0 & \text{for } x \in \partial(Q_l(i) \cap \mathcal{N}), \end{cases}$$

where $\rho_i := \rho + m_i$ and $J \subseteq \mathbb{N}$ is finite with $r_j > 0$ for $j \in J$. Since $|m_i| \leq \frac{\rho}{2}$, one has $\rho_i \in [\frac{1}{2}\rho, \frac{3}{2}\rho]$ for $i \in I$. Choose $(x_j)_{j\in J} \subset \mathcal{N}$ and $r_j > 0$ for $j \in J$ such that

$$\sum_{j\in J} |Q_l(i) \cap B_{r_j}| = \rho_i |Q_l(i) \cap \mathcal{N}|. \tag{3.35}$$

Therefore, there exists a solution to this boundary value problem.

Now, define the modified set $\tilde{\Omega} := (\Omega_{\rho,L} \cap \mathcal{O}) \cup \bigcup_{j\in J}(x_j + B_{r_j})$ and the modified vector field

$$\tilde{\mathbf{b}} := \begin{cases} \mathbf{b}_{\rho,L}(x) & \text{for } x \in \mathcal{O}, \\ -\boldsymbol{\nabla} u_i(x) - \boldsymbol{\nabla} v_i(x) & \text{for } x \in Q_l(i) \cap \mathcal{N}. \end{cases}$$

By definition $\tilde{\mathbf{b}} \cdot \nu$ is continuous on ∂Q_T, $\tilde{\mathbf{b}} \cdot \nu = 0$ on ∂Q_L and

$$\nabla \tilde{\mathbf{b}} = 1_{\tilde{\Omega}} - \rho \quad \text{in} \quad Q_L \backslash Q_R(a).$$

By equation (3.35) one has

$$\begin{aligned} |\tilde{\Omega}| &= |\Omega_{\rho,L} \cap \mathcal{O}| + \sum_{j\in J} |B_{r_j}| \\ &= \int_{\mathcal{O}} (1_{\Omega_{\rho,L}}(x) - \rho)\, \mathrm{d}x + \rho|\mathcal{O}| + \rho|\mathcal{N}| + \sum_{i\in I} m_i |Q_l(i) \cap \mathcal{N}|. \\ &= \rho|Q_L \backslash Q_R(a)| + \int_{\mathcal{O}} \nabla \mathbf{b}_{\rho,L}\, \mathrm{d}x - \sum_{i\in I} \int_{Q_l(i)\cap \partial Q_T} \mathbf{b}_{\rho,L} \cdot \nu\, \mathrm{d}x' \\ &= \rho |Q_L \backslash Q_R(a)|, \end{aligned}$$

because of the Neumann boundary condition $\mathbf{b}_{\rho,L} \cdot \nu = 0$ on ∂Q_L. Therefore, $(\tilde{\Omega}, \tilde{\mathbf{b}}) \in \mathcal{A}_{\mathrm{Neu}}(\rho, Q_L \backslash Q_R(a))$ and

$$\begin{aligned} & E_{\mathrm{Neu}}(\rho, Q_L \backslash Q_R(a)) \\ & \leq \mathcal{E}(\tilde{\Omega}, \tilde{\mathbf{b}}, Q_L \backslash Q_R(a)) \\ & = \mathrm{Per}(\Omega_{\rho,L} \cap \mathcal{O}) + \sum_{j\in J} \mathrm{Per}(B_{r_j}) + \frac{1}{2} \int_{\mathcal{O}} |\mathbf{b}_{\rho,L}|^2\, \mathrm{d}x + \frac{1}{2} \sum_{i\in I} \int_{Q_l(i)\cap\mathcal{N}} |\boldsymbol{\nabla} u_i + \boldsymbol{\nabla} v_i|^2\, \mathrm{d}x \\ & \leq \mathrm{Per}(\Omega_{\rho,L} \backslash Q_R(a)) + \frac{1}{2} \int_{Q_L \backslash Q_R(a)} |\mathbf{b}_{\rho,L}|^2\, \mathrm{d}x + \sum_{j\in J} \mathrm{Per}(B_{r_j}) + \sum_{i\in I} \int_{Q_l(i)\cap\mathcal{N}} |\boldsymbol{\nabla} u_i|^2\, \mathrm{d}x \\ & \quad + \sum_{i\in I} \int_{Q_l(i)\cap\mathcal{N}} |\boldsymbol{\nabla} v_i|^2\, \mathrm{d}x\,. \end{aligned}$$

The first two terms are just $\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_L \backslash Q_R(a))$. So it remains to estimate the other terms. As it is done in the proof of Lemma 3.12 choose $(x_j)_{j\in J} \subset \mathcal{N}$ and $r_j > 0$ for $j \in J$ such that

$$2 \sum_{j\in J} \mathrm{Per}(Q_l(i) \cap B_{r_j}) + \int_{Q_l(i)\cap\mathcal{N}} |\boldsymbol{\nabla} u_i|^2\, \mathrm{d}x \leq C c_{d,\rho} \rho |Q_l(i) \cap \mathcal{N}|. \tag{3.36}$$

Furthermore, with Lemma C.1 in [2] one has

$$\sum_{i\in I}\int_{Q_l(i)\cap\mathcal{N}}|\boldsymbol{\nabla} v_i|^2\,\mathrm{d}x \le \sum_{i\in I} Cl\int_{Q_l(i)\cap\partial Q_T(a)}|\mathbf{b}_{\rho,L}|^2\,\mathrm{d}x' \\ = Cl\int_{\partial Q_T(a)}|\mathbf{b}_{\rho,L}|^2\,\mathrm{d}x' \le C\frac{l}{\tilde{l}}S_{\rho,L}.$$

□

After proving uniform distribution of energy down to scale $Cc_{d,\rho}^{1/2}\rho^{-1/2}$, the bound on $S_{\rho,L}$ in the proof of Proposition 3.14 can be improved.

Corollary 3.18 (Uniform distribution of energy, Upper Bound)**.** *Let* $(\Omega_{\rho,L},\mathbf{b}_{\rho,L})$ *be a minimizer of* $\mathcal{E}(\cdot,\cdot,Q_L)$ *over* $\mathcal{A}_{\mathrm{Neu}}(\rho,Q_L)$*. If* $\rho\in(0,\frac{1}{2}]$ *and* $L\ge R\ge Cc_{d,\rho}^{1/2}\rho^{-1/2}$*, then one has for all* $a\in Q_L$ *such that* $Q_R(a)\subseteq Q_L$ *the local energy estimate*

$$\mathcal{E}(\Omega_{\rho,L},\mathbf{b}_{\rho,L},Q_R(a)) \le E_{\mathrm{Neu}}(\rho,Q_R(a)) + Cc_{d,\rho}^{(d+2)/(d+1)}\rho^{d/(d+1)}R^{d-2/(d+1)} \\ + 2\mathcal{H}^{d-1}(\Omega_{\rho,L}\cap\partial Q_R(a)\backslash\partial Q_L).$$

Proof. Instead of estimating $S_{\rho,L}\le Cc_{d,\rho}\rho R^d$ as in (3.33), one can estimate $S_{\rho,L}\le Cc_{d,\rho}\rho R^{d-1}\tilde{l}$ if $\tilde{l}\ge Cc_{d,\rho}^{1/2}\rho^{-1/2}$. In order to meet the condition $S_{\rho,L}<\frac{\rho^2}{2^{2d+3}}l^{d+1}\tilde{l}$ choose the parameters $l:=C_l c_{d,\rho}^{1/(d+1)}\rho^{-1/(d+1)}R^{1-2/(d+1)}$ and $\tilde{l}:=C_{\tilde{l}}C_l^{-1}l$ with $C_{\tilde{l}}\ge C_l>0$. Thus, it is deduced

$$E_{\mathrm{Neu}}(\rho,Q_L\backslash Q_R(a)) \le \mathcal{E}(\Omega_{\rho,L},\mathbf{b}_{\rho,L},Q_L\backslash Q_R(a)) + Cc_{d,\rho}\rho\,\tilde{l}R^{d-1} + C\frac{l}{\tilde{l}}S_{\rho,L} \\ \le \mathcal{E}(\Omega_{\rho,L},\mathbf{b}_{\rho,L},Q_L\backslash Q_R(a)) + Cc_{d,\rho}^{(d+2)/(d+1)}\rho^{d/(d+1)}R^{d-2/(d+1)},$$

if $R\ge\tilde{l}\ge Cc_{d,\rho}^{1/2}\rho^{-1/2}$. A simple calculation shows $\tilde{l}\ge Cc_{d,\rho}^{1/2}\rho^{-1/2}$ if $R\ge Cc_{d,\rho}^{1/2}\rho^{-1/2}$. □

Remark 3.19. In particular, if $R\ge C\delta^{-(d+1)/2}c_{d,\rho}^{1/2}\rho^{-1/2}$, this implies

$$\mathcal{E}(\Omega_{\rho,L},\mathbf{b}_{\rho,L},Q_R(a)) \le E_{\mathrm{Neu}}(\rho,Q_R(a)) + \delta c_{d,\rho}\rho R^d + 2\mathcal{H}^{d-1}(\Omega_{\rho,L}\cap\partial Q_R(a)\backslash\partial Q_L)$$

for any $\delta>0$. This is a significant improvement of the result of Proposition 3.14 which required $R\ge C\delta^{-(d+3/2)}c_{d,\rho}^{1/2}\rho^{-1/2}$.

3.2.2 Lower Bound on the Local Energy

Proposition 3.20 (Uniform distribution of energy, lower bound)**.** *Let* $(\Omega_{\rho,L},\mathbf{b}_{\rho,L})$ *be a minimizer of* $\mathcal{E}(\cdot,\cdot,Q_L)$ *over* $\mathcal{A}_{\mathrm{Neu}}(\rho,Q_L)$*. If* $\rho\in(0,\frac{1}{2}]$ *and* $L\ge R\ge Cc_{d,\rho}^{1/2}\rho^{-1/2}$*, then one has for all* $a\in Q_L$ *such that* $Q_R(a)\subseteq Q_L$ *the local energy estimate*

$$\mathcal{E}(\Omega_{\rho,L},\mathbf{b}_{\rho,L},Q_R(a)) \ge E_{\mathrm{Neu}}(\rho,Q_R(a)) - Cc_{d,\rho}^{(d+2)/(d+1)}\rho^{d/(d+1)}R^{d-2/(d+1)}. \qquad (3.37)$$

Proof. The lower bound is proven with the upper bound in Corollary 3.18 and the complementary case of Lemma 3.17. (Compare the outer case of Proposition 4.1 in [2].)

Lemma 3.21. *Let $\frac{1}{3}R \geq \tilde{l} \geq l \geq C$ for large $C > 0$ and assume*

$$T_{\rho,L} := \int_{(Q_{R-\tilde{l}}(a)\setminus Q_{R-2\tilde{l}}(a))} |\mathbf{b}_{\rho,L}|^2 \, \mathrm{d}x < \frac{\rho^2}{2^{2d+3}} l^{d+1}\tilde{l}. \tag{3.38}$$

Then,

$$E_{\mathrm{Neu}}(\rho, Q_R(a)) \leq \mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a)) + C c_{d,\rho}\rho\,\tilde{l}R^{d-1} + C\frac{l}{\tilde{l}}T_{\rho,L} \tag{3.39}$$

Choose $l := C_l c_{d,\rho}^{1/(d+1)} \rho^{-1/(d+1)} R^{1-2/(d+1)}$ and $\tilde{l} := C_{\tilde{l}} C_l^{-1} l$ with sufficiently large $C_{\tilde{l}} \geq C_l > 0$. The condition $\frac{1}{3}R \geq \tilde{l} \geq l$ is fulfilled since $R \geq C c_{d,\rho}^{1/2}\rho^{-1/2}$. By Proposition 3.14 one has

$$\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a)) \leq E_{\mathrm{Neu}}(\rho, Q_R(a)) + c_{d,\rho}\rho R^d + 2\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_R(a)\setminus\partial Q_L),$$

if $R \geq C c_{d,\rho}^{1/2}\rho^{-1/2}$. To get an estimate for the surface term, consider

$$\frac{1}{2}\int_R^{2R}\int_{\partial Q_T(a)} 1_{\Omega_{\rho,L}} \, \mathrm{d}x' \, \mathrm{d}T = \int_{Q_{2R}(a)\setminus Q_R(a)} 1_{\Omega_{\rho,L}} \, \mathrm{d}x \leq |Q_{2R}(a) \cap \Omega_{\rho,L}| \leq \rho^{1/2}R^d,$$

Here, the last inequality follows from Corollary **??**. Thus, there exists $T \in (R, 2R)$ such that

$$\mathcal{H}^{d-1}(\Omega_{\rho,L} \cap \partial Q_T(a)) = \int_{\partial Q_T(a)} 1_{\Omega_{\rho,L}} \, \mathrm{d}x' \leq 2\rho^{1/2}R^{d-1}.$$

Therefore, one can estimate

$$\begin{aligned} T_{\rho,L} &\leq \int_{Q_T(a)} |\mathbf{b}_{\rho,L}|^2 \, \mathrm{d}x \leq 2\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_T(a)) \\ &\leq C c_{d,\rho}\rho R^{d-1}\tilde{l} + 8\rho^{1/2}R^{d-1} \\ &\leq C c_{d,\rho}\rho R^{d-1}\tilde{l} \end{aligned} \tag{3.40}$$

if $\tilde{l} \geq C c_{d,\rho}^{1/2}\rho^{-1/2}$. Plugging this estimate in equation (3.39) gives

$$E_{\mathrm{Neu}}(\rho, Q_R(a)) \leq \mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a)) + C c_{d,\rho}^{(d+2)/(d+1)} \rho^{d/(d+1)} R^{d-2/(d+1)}.$$

This is inequality (3.37). □

Proof of Lemma 3.21. A straightforward adaption of the proof of Lemma 3.17 works in this complementary case. This is why this proof is only sketched. (See also the proof of Proposition 4.1 in [2].) Let $\mathcal{O} := Q_T(a)$ and $\mathcal{N} := Q_R(a)\setminus\overline{Q_T(a)}$. Since

$$\frac{1}{2}\int_{R-2\tilde{l}}^{R-\tilde{l}}\int_{\partial Q_T(a)} |\mathbf{b}_{\rho,L}|^2 \, \mathrm{d}x' \, \mathrm{d}T = T_{\rho,L}$$

there exists a $T \in [R-2\tilde{l}, R-\tilde{l}]$ such that

$$\int_{\partial Q_T(a)} |\mathbf{b}_{\rho,L}|^2 \,\mathrm{d}x' \leq \frac{2}{\tilde{l}} T_{\rho,L}. \tag{3.41}$$

As in the proof of Lemma 3.17, define the modified set $\tilde{\Omega} := (\Omega_{\rho,L} \cap \mathcal{O}) \cup \bigcup_{j\in J}(x_j + B_{r_j})$ and the modified vector field

$$\tilde{\mathbf{b}} := \begin{cases} \mathbf{b}_{\rho,L}(x) & \text{for } x \in \mathcal{O}, \\ -\nabla u(x) - \nabla v_i(x) & \text{for } x \in Q_l(i) \cap \mathcal{N}, \end{cases}$$

such that $(\tilde{\Omega}, \tilde{\mathbf{b}}) \in \mathcal{A}_{\mathrm{Neu}}(\rho, Q_R(a))$. Then, one can bound the energy from above

$$\begin{aligned} &E_{\mathrm{Neu}}(\rho, Q_R(a)) \leq \mathcal{E}(\tilde{\Omega}, \tilde{\mathbf{b}}, Q_R(a)) \\ &= \mathrm{Per}(\Omega_{\rho,L} \cap \mathcal{O}) + \sum_{j\in J} \mathrm{Per}(B_{r_j}) + \frac{1}{2}\int_{\mathcal{O}} |\mathbf{b}_{\rho,L}|^2 \,\mathrm{d}x + \frac{1}{2}\sum_{i\in I}\int_{Q_l(i)\cap\mathcal{N}} |\nabla u + \nabla v_i|^2 \,\mathrm{d}x \\ &\leq \mathrm{Per}(\Omega_{\rho,L} \cap Q_R(a)) + \frac{1}{2}\int_{Q_R(a)} |\mathbf{b}_{\rho,L}|^2 \,\mathrm{d}x + \sum_{j\in J}\mathrm{Per}(B_{r_j}) + \int_{\mathcal{N}} |\nabla u|^2 \,\mathrm{d}x + \sum_{i\in I}\int_{Q_l(i)\cap\mathcal{N}} |\nabla v_i|^2 \,\mathrm{d}x\,. \end{aligned}$$

The first two terms are just $\mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_R(a))$. The remaining terms are estimated as in the proof Lemma 3.17. □

3.3 Existence of the Thermodynamic Limit

The existence of the thermodynamic limit is not assumed when the uniform distribution of energy is derived in the previous sections. This existence and its equality for several boundary conditions can easily be proven based on uniform distribution of energy.

Theorem 3.22 (Thermodynamic limit)**.** *For $\rho \in (0, \frac{1}{2}]$, there exists $e_0(\rho) \in \mathbb{R}$, such that for any given boundary condition $\# \in \{\mathrm{Dir}, \infty, \mathrm{Neu}\}$ one has for $L \geq C c_{d,\rho}^{1/2} \rho^{-1/2}$*

$$\left| \frac{1}{L^d} E_\#(\rho, Q_L) - e_0(\rho) \right| \leq \frac{C}{L^{1/(d+3/2)}}. \tag{3.42}$$

In particular, the thermodynamic limit exists and is the same for these boundary conditions.

Note that the constant $C > 0$ does not depend on ρ. Rescaling the energy defined in terms of the electric field $E_\#(\rho, Q_L)$ gives the energy defined in terms of the Coulomb potential $E^\#_{\rho,L}$. Indeed,

$$\lim_{L\to\infty} \frac{1}{L^d} E_\#(\rho, Q_L) = \frac{1}{c_d^{1/3}} \lim_{L\to\infty} \frac{1}{L^d} E^\#_{\rho,L}.$$

Here, $c_2 = 2\pi$ and $c_d = (d-2)|\mathbb{S}^{d-1}|$ as defined in the introduction. (It should not be confused with $c_{d,\rho}$.)

Remark 3.23. A future project might be to improve to the error in this estimate with the method used by Armstrong and Serfaty in [2]. For this purpose one has to prove estimates for the minimizer of the Dirichlet energy.

Remark 3.24. As explained in Section 1.4 in the introduction the energy of any boundary condition with a potential $v_{\rho,L}$ of the minimizer $\Omega_{\rho,L}$ fulfilling

$$\int_{\partial Q_L} v_{\rho,L}\, \nu \cdot \boldsymbol{\nabla} v_{\rho,L} \,\mathrm{d}x' \leq 0 \tag{3.43}$$

can be bounded from above by the Neumann energy and from below by the Dirichlet energy. Therefore, the thermodynamic limit exists by the theorem above and is equal to $e_0(\rho)$. In particular, this includes periodic boundary conditions.

In this section the existence of the thermodynamic limit and its equality for several boundary conditions is proven based on uniform distribution of energy. Parts of it are similar to the proofs of Lemma 3.1 and Lemma 3.10 in [1].

Proof of Theorem 3.22. The proof progresses in four steps. First of all, the super-additivity of the Dirichlet energy and the sub-additivity of the Neumann energy imply their monotonicity for the limit $nL_0 \to \infty$ as $n \to \infty$ for $n \in \mathbb{N}$ (see Lemma 3.1 in [1]). Secondly, it is shown that subsequences of these limits actually achieve the limit superior and the limit inferior. Then, the existence of the thermodynamic limit is concluded (compare Lemma 3.10 in [1]) assuming that the Neumann energy can be bounded from above by the Dirichlet energy. Finally, this remaining inequality is deduced. Note that this fourth step is crucial since it is only known that the Dirichlet energy can be bounded from above by the Neumann energy by inequality (1.14). Here, the proof is based on the method used by Armstrong and Serfaty in [2] which is different to what is done by [1].

Step 1. Monotonicity of the Dirichlet and of the Neumann energy Clearly, $E_{\mathrm{Dir}}(\rho, Q_L) \leq E_{\mathrm{Neu}}(\rho, Q_L)$. Let $n \in (2\mathbb{N}+1)$. Then

$$\frac{1}{n^d L^d} E_{\mathrm{Dir}}(\rho, Q_{nL}) \geq \frac{1}{L^d} E_{\mathrm{Dir}}(\rho, Q_L) - \frac{C}{L}. \tag{3.44}$$

Indeed, suppose $(\Omega, \mathbf{b})$ is a minimizer of $\mathcal{E}$ over $\mathcal{A}_{\mathrm{Dir}}(\rho, Q_{nL})$. Then

$$\begin{aligned}
E_{\mathrm{Dir}}(\rho, Q_{nL}) &= \mathcal{E}(\Omega, \mathbf{b}, Q_{nL}) = \mathrm{Per}(\Omega) + \frac{1}{2}\int_{Q_{nL}} |\mathbf{b}|^2 \,\mathrm{d}x \\
&\geq \sum_{r \in L\mathbb{Z}^d} \mathrm{Per}(\Omega \cap Q_L(r)) - Cn^d L^{d-1} + \sum_{r \in L\mathbb{Z}^d} \int_{Q_L(r)} |\mathbf{b}|^2 \,\mathrm{d}x \\
&= \sum_{r \in L\mathbb{Z}^d} \mathcal{E}(\Omega, \mathbf{b}, Q_L(r)) - Cn^d L^{d-1} \\
&\geq n^d \inf_{r \in L\mathbb{Z}^d} \mathcal{E}(\Omega, \mathbf{b}, Q_L(r)) - Cn^d L^{d-1} \\
&\geq n^d E_{\mathrm{Dir}}(\rho, Q_L) - Cn^d L^{d-1},
\end{aligned}$$

since the energy is translation invariant. So the Dirichlet energy is increasing.

Similarly, for $n \in (2\mathbb{N}+1)$, one has

$$\frac{1}{n^d L^d} E_{\mathrm{Neu}}(\rho, Q_{nL}) \leq \frac{1}{L^d} E_{\mathrm{Neu}}(\rho, Q_L) + \frac{C}{L} \tag{3.45}$$

since n^d copies of the minimizer $(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}) \in \mathcal{A}_{\mathrm{Neu}}(\rho, Q_L)$ can be glued together. Indeed, let $\tilde{\Omega} := \bigcup_{r \in L\mathbb{Z}^d, |r|_\infty \leq n} (\Omega_{\rho,L} + r)$ and let $\tilde{\mathbf{b}}(x) := \mathbf{b}_{\rho,L}(x - r)$ for $x \in Q_L(r)$ and $r \in L\mathbb{Z}^d$ with $|r|_\infty \leq n$. This construction fulfills the Neumann boundary condition, that is $(\tilde{\Omega}, \tilde{\mathbf{b}}) \in \mathcal{A}_{\mathrm{Neu}}(\rho, Q_{nL})$. Therefore,

$$E_{\mathrm{Neu}}(\rho, Q_{nL}) \leq \mathcal{E}(\tilde{\Omega}, \tilde{\mathbf{b}}, Q_{nL}) \leq n^d \mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_L) + n^d L^{d-1} = n^d E_{\mathrm{Neu}}(\rho, Q_L) + n^d L^{d-1}.$$

So the Neumann energy is decreasing.

Step 2. It is sufficient to consider the sequence nL_0 Let $L_0 > C c_{d,\rho}^{1/2} \rho^{-1/2}$. Define the limit superior and the limit inferior of the ground state energy

$$e_-^{\#}(\rho) := \liminf_{n\to\infty} \frac{1}{n^d L_0^d} E_{\#}(\rho, Q_{nL_0}) \quad \text{and} \quad e_+^{\#}(\rho) := \limsup_{n\to\infty} \frac{1}{n^d L_0^d} E_{\#}(\rho, Q_{nL_0}), \tag{3.46}$$

for $\# \in \{\mathrm{Dir}, \mathrm{Neu}\}$. Since $E_{\mathrm{Dir}}(\rho, Q_L) \leq E_{\mathrm{Neu}}(\rho, Q_L)$, trivially

$$e_\pm^{\mathrm{Dir}}(\rho) \leq e_\pm^{\mathrm{Neu}}(\rho).$$

The goal of the next part of the proof is to show

$$e_+^{\mathrm{Neu}}(\rho) = \limsup_{L\to\infty} \frac{1}{L^d} E_{\mathrm{Neu}}(\rho, Q_L) \quad \text{and} \quad e_-^{\mathrm{Neu}}(\rho) = \liminf_{L\to\infty} \frac{1}{L^d} E_{\mathrm{Neu}}(\rho, Q_L). \tag{3.47}$$

In particular, $e_\pm^{\mathrm{Neu}}(\rho)$ is not dependent on L_0.

Let $(L_k)_{k\in\mathbb{N}}$ be a strictly increasing sequence in $(0,\infty)$ with $L_k \to \infty$ $(k \to \infty)$ such that $\limsup_{L\to\infty} \frac{1}{L^d} E_{\mathrm{Neu}}(\rho, Q_L) = \lim_{k\to\infty} \frac{1}{L_k^d} E_{\mathrm{Neu}}(\rho, Q_{L_k})$. For any $k \in \mathbb{N}$ there exists $n_k \in \mathbb{N}$ such that $L_k \in [n_k L_0, (n_k+1)L_0]$. By Theorem 3.8 one has

$$\begin{aligned}
\frac{1}{L_k^d} E_{\mathrm{Neu}}(\rho, Q_{L_k}) &= \frac{1}{L_k^d} \mathcal{E}(\Omega_{\rho,L_k}, \mathbf{b}_{\rho,L_k}, Q_{L_k}) \\
&= \frac{1}{L_k^d} \mathcal{E}(\Omega_{\rho,L_k}, \mathbf{b}_{\rho,L_k}, Q_{n_k L_0}) + \frac{1}{L_k^d} \mathcal{E}(\Omega_{\rho,L_k}, \mathbf{b}_{\rho,L_k}, Q_{L_k} \backslash Q_{n_k L_0}) + \mathcal{O}\Big(L_k^{-1}\Big) \\
&= \frac{1}{n_k^d L_0^d} E_{\mathrm{Neu}}(\rho, Q_{n_k L_0}) + \mathcal{O}\Big(L_k^{-2/(d+1)}\Big).
\end{aligned}$$

The energy on $Q_{L_k} \backslash Q_{n_k L_0}$ is estimated $0 \leq \mathcal{E}(\Omega_{\rho,L_k}, \mathbf{b}_{\rho,L_k}, Q_{L_k} \backslash Q_{n_k L_0}) \leq C c_{d,\rho}^{1/2} \rho (L_k^d - n_k^d L_0^d)$ by uniform distribution of energy. Note that $n_k^d L_0^d = L_k^d + \mathcal{O}(L_0 L_k^{d-1})$. Therefore,

$$\begin{aligned}
\limsup_{L\to\infty} \frac{1}{L^d} E_{\mathrm{Neu}}(\rho, Q_L) &= \lim_{k\to\infty} \frac{1}{L_k^d} E_{\mathrm{Neu}}(\rho, Q_{L_k}) = \lim_{k\to\infty} \frac{1}{n_k^d L_0^d} E_{\mathrm{Neu}}(\rho, Q_{n_k L_0}) \\
&\leq e_+^{\mathrm{Neu}}(\rho) \leq \limsup_{L\to\infty} \frac{1}{L^d} E_{\mathrm{Neu}}(\rho, Q_L).
\end{aligned}$$

This proves the limit superior equality in equation (3.47) and shows $e_+^{\mathrm{Neu}}(\rho)$ is not dependent on L_0. Similarly, for a sequence $(\tilde{L}_k)_{k\in\mathbb{N}}$ that achieves the limit inferior it can be estimated

$$\begin{aligned}\liminf_{L\to\infty}\frac{1}{L^d}E_{\mathrm{Neu}}(\rho,Q_L) &= \lim_{k\to\infty}\frac{1}{\tilde{L}_k^d}E_{\mathrm{Neu}}(\rho,Q_{\tilde{L}_k}) = \lim_{k\to\infty}\frac{1}{\tilde{n}_k^d L_0^d}E_{\mathrm{Neu}}(\rho,Q_{n_k L_0})\\ &\geq e_-^{\mathrm{Neu}}(\rho) \geq \liminf_{L\to\infty}\frac{1}{L^d}E_{\mathrm{Neu}}(\rho,Q_L).\end{aligned}$$

Of course, $\tilde{n}_k\in\mathbb{N}$ is chosen such that $\tilde{L}_k\in[\tilde{n}_k L_0,(\tilde{n}_k+1)L_0]$ and uniform distribution of energy is applied.

Step 3. Concluding the proof Later it will be shown

$$\frac{1}{L^d}E_{\mathrm{Neu}}(\rho,Q_L) \leq \frac{1}{L^d}E_{\mathrm{Dir}}(\rho,Q_L) + \frac{C}{L^{1/(d+3/2)}}. \tag{3.48}$$

The super-additivity of the Dirichlet energy (3.44) and the sub-additivity of the Neumann energy (3.45) imply the estimates

$$e_\pm^{\mathrm{Dir}}(\rho) \geq \frac{1}{L^d}E_{\mathrm{Dir}}(\rho,Q_L) - \frac{C}{L} \quad\text{and}\quad e_\pm^{\mathrm{Neu}}(\rho) \leq \frac{1}{L^d}E_{\mathrm{Neu}}(\rho,Q_L) + \frac{C}{L}. \tag{3.49}$$

Therefore, by inequality (3.48) it follows

$$e_+^{\mathrm{Neu}}(\rho) \leq e_-^{\mathrm{Dir}}(\rho) \leq e_-^{\mathrm{Neu}}(\rho) \leq e_+^{\mathrm{Neu}}(\rho). \tag{3.50}$$

In particular, $e_-^{\mathrm{Dir}}(\rho)$ does not depend on L_0 and $\lim_{L\to\infty}\frac{1}{L^d}E_{\mathrm{Neu}}(\rho,Q_L) = e_-^{\mathrm{Neu}}(\rho) = e_+^{\mathrm{Neu}}(\rho) =: e_0(\rho)$. Furthermore, $e_+^{\mathrm{Neu}}(\rho) \leq e_+^{\mathrm{Dir}}(\rho) \leq e_+^{\mathrm{Neu}}(\rho)$. In particular, $e_+^{\mathrm{Dir}}(\rho)$ does not depend on L_0. Then, inequalities (3.48) and (3.49) can be combined to get

$$e_+^{\mathrm{Dir}}(\rho) \leq e_+^{\mathrm{Neu}}(\rho) \leq \frac{1}{L^d}E_{\mathrm{Dir}}(\rho,Q_L) + \frac{C}{L^{1/(d+3/2)}} \leq e_+^{\mathrm{Dir}}(\rho) + \frac{C}{L^{1/(d+3/2)}}.$$

This implies $\lim_{L\to\infty} E_{\mathrm{Dir}}(\rho,Q_L) = e_+^{\mathrm{Dir}}(\rho) = e_0(\rho)$.

Step 4. Proving the remaining inequality Let $(\Omega_{\rho,L},\mathbf{b}_{\rho,L})$ be the minimizer of $\mathcal{E}(\cdot,\cdot,Q_L)$ over $\mathcal{A}_{\mathrm{Dir}}(\rho,Q_L)$. To show

$$E_{\mathrm{Dir}}(\rho,Q_L) \geq E_{\mathrm{Neu}}(\rho,Q_L) - Cc_{d,\rho}^{1+1/(2d+3)}\rho^{1-1/(2d+3)}L^{d-1/(d+3/2)},$$

let $l\leq\tilde{l}\leq\frac{1}{3}R$ and $T\in(R-2\tilde{l},R-\tilde{l})$ be such that

$$\frac{\tilde{l}}{2}\int_{\partial Q_T}|\mathbf{b}_{\rho,L}|^2\,\mathrm{d}x' \leq T_{\rho,L}^{\mathrm{Dir}} := \int_{Q_{R-\tilde{l}}(a)\setminus Q_{R-2\tilde{l}}(a)}|\mathbf{b}_{\rho,L}|^2\,\mathrm{d}x \tag{3.51}$$

Define the old region $\mathcal{O} := Q_T$ that is not changed and the new region $\mathcal{N} := Q_L\setminus Q_T$ that is changed. Exactly as in the proof of uniform distribution of energy choose $(x_j)_{j\in J}\subset\mathcal{N}$

and $r_j > 0$ such that $\sum_{j\in J} |B_{r_j}(x_j) \cap Q_l(i)| = (\rho + m_i)|Q_l(i) \cap \mathcal{N}|$ where $\mathcal{N}$ is partitioned into rectangles $Q_l(i) \cap \mathcal{N}$ for $i \in I := \{k \in l\mathbb{Z}^d : k \in \mathcal{N}\}$. It is assumed that the constant $C_l > 0$ is chosen such that $\partial Q_T(a) \subset \sum_{i\in I} \overline{Q_l(i)}$. Furthermore,

$$m_i := -(|Q_l(i) \cap \mathcal{N}|)^{-1} \int_{Q_l(i)\cap\partial Q_T} \mathbf{b}_{\rho,L} \cdot \nu \,\mathrm{d}x' .$$

Let $u_i \in H^2(\mathcal{N})$ be the solution with mean zero of $-\Delta u = \sum_j 1_{B_{r_j}(x_j)} - (\rho + m_i)$ in $Q_l(i) \cap \mathcal{N}$ and $\nu \cdot \boldsymbol{\nabla} u_i = 0$ on $\partial(Q_l(i) \cap \mathcal{N})$. Furthermore, let $v_i \in H^2(Q_l(i) \cap \mathcal{N})$ be the solution with mean zero of $-\Delta v_i = m_i$ in $Q_l(i) \cap \mathcal{N}$ and $\nu \cdot \boldsymbol{\nabla} v_i = g$ on $\partial(Q_l(i) \cap \mathcal{N})$ where $g = \nu \cdot \mathbf{b}_{\rho,L}$ on ∂Q_T and $g = 0$ otherwise.

Define $\Omega := (\Omega_{\rho,L} \cap \mathcal{O}) \cup \bigcup_{j\in J} B_{r_j}(x_j)$ and

$$\mathbf{b}(x) := \begin{cases} \mathbf{b}_{\rho,L}(x) & \text{for } x \in \mathcal{O}, \\ -\boldsymbol{\nabla} u_i - \boldsymbol{\nabla} v_i & \text{for } x \in Q_l(i) \cap \mathcal{N}. \end{cases}$$

This implies

$$\begin{aligned} |\Omega| &= |\Omega_{\rho,L} \cap \mathcal{O}| + \sum_{j\in J} |B_{r_j}| \\ &= \int_{\mathcal{O}} (1_{\Omega_{\rho,L}}(x) - \rho) \,\mathrm{d}x + \rho|\mathcal{O}| + \rho|\mathcal{N}| + \sum_{i\in I} m_i |Q_l(i) \cap \mathcal{N}| \\ &= \rho|Q_L \backslash Q_R(a)| + \int_{\mathcal{O}} \boldsymbol{\nabla} \mathbf{b}_{\rho,L} \,\mathrm{d}x - \sum_{i\in I} \int_{Q_l(i)\cap\partial Q_T} \mathbf{b}_{\rho,L} \cdot \nu \,\mathrm{d}x' \\ &= \rho L^d. \end{aligned}$$

Then, $|\Omega| = \rho L^d$, $\mathbf{b} \cdot \nu$ is continuous on ∂Q_T and $\mathbf{b} \cdot \nu = 0$ on ∂Q_L. Therefore $(\Omega, \mathbf{b}) \in \mathcal{A}_{\mathrm{Neu}}(\rho, Q_L)$ which implies

$$\begin{aligned} &E_{\mathrm{Neu}}(\rho, Q_L) \le \mathcal{E}(\Omega, \mathbf{b}, Q_L) \\ &\le \mathcal{E}(\Omega_{\rho,L}, \mathbf{b}_{\rho,L}, Q_T(a)) + \sum_j \mathrm{Per}(B_{r_j}) + \sum_i \int_{Q_l(i)\cap\mathcal{N}} |\boldsymbol{\nabla} u_i|^2 \,\mathrm{d}x + \sum_i \int_{Q_l(i)\cap\mathcal{N}} |\boldsymbol{\nabla} v_i|^2 \,\mathrm{d}x \\ &\le E_{\mathrm{Dir}}(\rho, Q_L) + C c_{d,\rho} \rho R^{d-1} \tilde{l} + C \frac{l}{\tilde{l}} T^{\mathrm{Dir}}_{\rho,L}. \end{aligned}$$

Lemma C.1 in [2] states that $\int_{Q_l(i)\cap\mathcal{N}} |\boldsymbol{\nabla} v_i|^2 \,\mathrm{d}x \le Cl \int_{\partial(Q_l(i)\cap\mathcal{N})} |g|^2 \,\mathrm{d}x'$.

By inequality (1.14) the Dirichlet energy can be estimated $T^{\mathrm{Dir}}_{\rho,L} \le E_{\mathrm{Dir}}(\rho, Q_L) \le E_\infty(\rho, Q_L) \le C c_{d,\rho} \rho L^d$. Therefore, $E_{\mathrm{Neu}}(\rho, Q_L) \le E_{\mathrm{Dir}}(\rho, Q_L) + C c_{d,\rho} \rho L^{d-1} \tilde{l} + C \frac{l}{\tilde{l}} c_{d,\rho} \rho L^d$. Minimizing over $\tilde{l}$ gives $\tilde{l} \propto \sqrt{lL}$. To fulfill the condition $T^{\mathrm{Dir}}_{\rho,L} \le 2^{-2d-3} \rho^2 \tilde{l} l^{d+1} = \frac{\rho^2}{C} \sqrt{L} l^{d+3/2}$ choose $l := C_l c_{d,\rho}^{1/(d+3/2)} \rho^{-1/(d+3/2)} R^{1-2/(d+3/2)}$ and $\tilde{l} := C_{\tilde{l}} c_{d,\rho}^{1/(2d+3)} \rho^{-1/(2d+3} L^{1-1/(d+3/2)}$ with $C_{\tilde{l}} \ge C_l > 0$. This condition ensures $m_i \in (\frac{1}{2}\rho, \frac{3}{2}\rho)$. Then

$$E_{\mathrm{Neu}}(\rho, Q_L) \le E_{\mathrm{Dir}}(\rho, Q_L) + C c_{d,\rho}^{1+1/(2d+3)} \rho^{1-1/(2d+3)} L^{d-1/(d+3/2)}. \tag{3.52}$$

□

Chapter 4

Large Polaron Systems and Bogolubov Theory

In this chapter a lower bound on the energy of a polaron system in the Pekar-Tomasevich approximation is proven. The idea is to linearize the energy and then, to estimate the Hamiltonian of this linearized energy from below. To make this precise, recall that a system of N polarons in the Pekar-Tomasevich approximation is described by

$$\mathcal{E}_1^{(N)}[\psi] = \int_{(\mathbb{R}^3)^N} \left(\sum_{i=1}^N |\boldsymbol{\nabla}_i \psi|^2 + \sum_{1 \le i < j \le N} \frac{|\psi|^2}{|x_i - x_j|} \right) \mathrm{d}x - D(\rho_\psi, \rho_\psi), \tag{4.1}$$

where $\psi \in H^1((\mathbb{R}^3)^N)$ is symmetric with $\int_{(\mathbb{R}^3)^N} |\psi|^2 \, \mathrm{d}x = 1$. Furthermore, the one-particle density is

$$\rho_\psi(z) = \sum_{i=1}^N \int \cdots \int_{(\mathbb{R}^3)^{(N-1)}} |\psi(x_1, \ldots, x_{i-1}, z, x_{i+1}, \ldots, x_N)|^2 \, \mathrm{d}x_1 \ldots \mathrm{d}x_{i-1} \, \mathrm{d}x_{i+1} \ldots \mathrm{d}x_N \tag{4.2}$$

for $z \in \mathbb{R}^3$ and the attractive term is

$$D(\rho_1, \rho_2) := \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\overline{\rho_1(y)} \rho_2(z)}{|y - z|} \, \mathrm{d}y \, \mathrm{d}z \, . \tag{4.3}$$

In this chapter the following lower bound on the corresponding ground state energy $E_1^{(\mathrm{b})}(N)$ is proven.

Theorem 4.1. *The ground state energy of a Pekar-Tomasevich polaron system in the many particle limit is bounded from below as*

$$\liminf_{N \to \infty} N^{-7/5} E_1^{(\mathrm{b})}(N) \ge -A, \tag{4.4}$$

where

$$A = \inf \left\{ \int_{\mathbb{R}^3} |\boldsymbol{\nabla} \phi|^2 \, \mathrm{d}x + I_0 \int_{\mathbb{R}^3} |\phi|^{5/2} \, \mathrm{d}x : \phi \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |\phi|^2 \, \mathrm{d}x \le 1 \right\}$$

and

$$I_0 = \frac{2}{5}\left(\frac{2}{\pi}\right)^{1/4}\frac{\Gamma(3/4)}{\Gamma(5/4)} \approx 0.6.$$

Remark 4.2. Theorem 1.7 stated in the introduction follows from this theorem and the corresponding upper bound proven by Benguria, Frank and Lieb [3, Theorem 1.1].

Since the proof is based on estimating the Hamiltonian of the linearized energy, a one component charged Bose gas with a background distribution of opposite charge is considered. This is why Bogolubov theory can be applied to derive the leading order. The approach is a mixture of what Lieb and Solovej do to prove lower bounds on the energy of a one component charged Bose gas with constant background [36] and of a two component charged Bose gas [37].

4.1 Proof of the Main Result and Outline of the Chapter

As it is done in [3], the non-linear energy of the polaron system can be expressed in terms of the infimum of a linear ground state energy over all backgrounds σ

$$E_1^{(\mathrm{b})}(N) = \inf_{\sigma} \inf \operatorname{spec} H^{(N)}, \tag{4.5}$$

for the Hamiltonian of a charged Bose gas

$$H^{(N)} := \sum_{i=1}^{N} - \Delta_i + \sum_{i<j} \frac{1}{|x_i - x_j|} - \sum_{i=1}^{N} \int_{\mathbb{R}^3} \frac{\sigma(y)}{|y - x_i|}\, \mathrm{d}y + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\sigma(y)\sigma(z)}{|y-z|}\, \mathrm{d}y\, \mathrm{d}z\,, \tag{4.6}$$

with background $\sigma \in L^1(\mathbb{R}^3)$ such that $D(\sigma,\sigma) < \infty$. The linearization formula (4.5) follows from the inequality

$$\left(\psi, H^{(N)}\psi\right) = \mathcal{E}_1^{(N)}[\psi] + D(\rho_\psi - \sigma, \rho_\psi - \sigma) \,\geq\, \mathcal{E}_1^{(N)}[\psi],$$

which holds since the Fourier transform of the Coulomb potential is positive.

After linearization, one has the quantum mechanical jellium model with a background charge density similar to [36]. Unlike there, the background σ is not fixed to be the indicator function $\rho 1_{Q_L}$ for some $\rho > 0$. On the contrary, the infimum is taken over all possible background distributions which makes this problem more similar to the two component charged Bose gas treated by Lieb and Solovej in [37].

Similar to [37], the proof proceeds in three main steps.

1. Localizing the Hamiltonian to small cubes of length $l \propto N^{-2/5+\delta_l}$ for a small $\delta_l > 0$.

2. Bounding the energy on a small cube from below.

3. Putting the small cubes together to get a lower bound for the whole space problem.

To state the localization result, define the Hamiltonian acting on functions on the small cube about kl,

$$\begin{aligned}\tilde{H}^{(k)} =& \gamma_{\varepsilon,t} \sum_{i=1}^{N} \left(\mathcal{K}_i^{(k)} - \varepsilon\, \Delta_{i,\mathrm{Neu}}^{(k)} \right) + \sum_{1\le i<j\le N} w_R^{(k)}(x_i, x_j) \\ &- \sum_{i=1}^{N} \int_{\mathbb{R}^3} \sigma(y) w_R^{(k)}(y, x_i)\, \mathrm{d}y + \frac{1}{2} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \sigma(y) w_R^{(k)}(y,z)\sigma(z)\, \mathrm{d}y\, \mathrm{d}z\,,\end{aligned}$$

where $\gamma_{\varepsilon,t} \to 1$ as $\varepsilon, t \to 0$ and where the interaction is given by

$$w_R^{(k)}(y,z) = \chi_l^{(k)}(y) \frac{\mathrm{e}^{-|y-z|/R}}{|y-z|} \chi_l^{(k)}(z). \tag{4.7}$$

Here, $\chi_l^{(k)}$ is a localization function in $C_{\mathrm{c}}^4(\mathbb{R}^3)$ which tends to the indicator function $1_{Q_l(kl)}$ if the localization parameter $t \to 0$ as explained in Section A.1. The long distance cutoff $R \le l$ is defined in (4.11).

The first theorem gives a lower bound of $E_1^{(\mathrm{b})}(N)$ in terms of this Hamiltonian $\tilde{H}^{(k)}$ on $Q_l(kl)$. Since one can use exactly the same procedure of localizing the Hamiltonian as in [37] (see also [36]), its proof is postponed to the appendix.

Theorem 4.3 (Localization to length scale $l \propto N^{-2/5+\delta_l}$). *The ground state energy of the polaron system is bounded below as*

$$\begin{aligned}E_1^{(\mathrm{b})}(N) \ge& \gamma\tilde{\gamma} \inf \left\{ \gamma_{\varepsilon,t}\, T(S_0^{\psi}) + \inf_{\sigma} \sum_{k\in\mathbb{Z}^3} \left(\psi, \tilde{H}^{(k)} \psi \right) :\ \psi \in \mathcal{H}_0 \text{ with } \|\psi\| = 1 \right\} \\ &- L^3 l^{-5} - Ct^{-4} N l^{-1} - N^{7/5}\left(Ct^{-2}(N^{1/5}L)^{-2} + Ct^{-4}(N^{1/5}L)^{-1}N^{-1/5} \right).\end{aligned}$$

where $\gamma, \tilde{\gamma} \to 1$ as $t \to 0$. The wave function ψ is in the space

$$\mathcal{H}_0 := \left\{ \phi \in \bigotimes\nolimits_{\mathrm{s}}^{N} L^2(\mathbb{R}^3) \;\middle|\; \hat{n}^{(k)}\phi = 0 \text{ for } kl \notin \mathbb{Z}^3 \cap Q_{L+l} \right\}.$$

where $L \propto N^{-1/5+\delta_L}$ for a small $\delta_L > 0$.

Here, $T(S_0^{\psi})$ is a discrete kinetic energy of ψ which is defined in equations (A.7) and (A.8) in the appendix. Its particular form is not needed for now. Furthermore, the particle number operator in the k-th small cube is given by

$$\hat{n}^{(k)}(x) = \sum_{i=1}^{N} 1_{Q_l(kl)}(x_i),$$

where $x \in (\mathbb{R}^3)^N$ and where 1_{Q_l} is the characteristic function of the cube $Q_l = (-l/2, l/2)^3$.

Define the number of particles in the condensate which are in the cube about kl

$$\hat{n}_0^{(k)} = l^{-3} a^*(1_{Q_l(kl)})\, a(1_{Q_l(kl)}),$$

where, for $u \in L^2(\mathbb{R}^3)$, the operators $a(u)$ and $a^*(u)$ act on the Fock space $\mathcal{F}_{\text{sym}}(L^2(\mathbb{R}^3)) = \bigoplus_{N=0}^{\infty} \bigotimes_{\text{sym}}^{N} L^2(\mathbb{R}^3)$ as defined in the introduction. Furthermore, define the number of excited particles in the k-th cube

$$\hat{n}_+^{(k)} = \hat{n}^{(k)} - \hat{n}_0^{(k)}.$$

The next step is to get a lower bound on $\tilde{H}^{(k)}$. On this small scale most particles are in the constant state, i.e. there is condensation. Similar to [36], Bogolubov theory will be used to calculate the leading order contribution to the ground state energy. The main difference is that one cannot get neutrality uniformly in space because of the background $\sigma \in L^1(\mathbb{R}^3)$. Instead, an approximate neutrality is proven in a local version of the Coulomb norm $\sqrt{D(\sigma, \sigma)}$.

The remaining Sections 4.2-4.7 are devoted to prove the following theorem.

Theorem 4.4 (Lower bound on the local energy)**.** *For eigenstates ψ of $\hat{n}^{(k)}$ with eigenvalue $n^{(k)}$, one has the following estimate for the Hamiltonian*

$$\begin{aligned} \left\langle \tilde{H}^{(k)} \right\rangle \geq & - \left\langle \hat{n}_0^{(k)} \right\rangle^{5/4} l^{-3/4} \Big(\gamma_{\varepsilon,t}^{-1/4} I_0 + CK(\varepsilon, t, N, l) \Big) \\ & - \left\langle \hat{n}_0^{(k)} \right\rangle^{5/3} l^{-1/3} (N^{2/5} l)^{-5/3} \Big(C\varepsilon^{1/6} + CK(\varepsilon, t, N, l) \Big) \\ & - C\varepsilon^{-1} t^{-6} n^{(k)} l^{-1} - Ct^{-22} l^{-2} - C\varepsilon^{-1} t^{-8} n^{(k)}. \end{aligned}$$

Here, $K(\varepsilon, t, N, l) = C \sum_{i=1}^{m} \varepsilon^{-a_i} t^{-b_i} (N^{2/5} l)^{c_i} N^{-d_i}$ with $d_i > 0$ for all i and $m \in \mathbb{N}$.

The final step is putting together the locally constant condensate particle numbers $\langle \hat{n}_0^{(k)} \rangle$ into one wave function $\tilde{\phi} \in H^1(\mathbb{R}^3)$ with the right properties. This work is already done in [37]. Therefore, the result of section 12 of [37] is quoted.

Theorem 4.5. *There exists a real valued $\tilde{\phi} \in H^1(\mathbb{R}^3)$ with compact support such that*

$$T(S_0^{\psi}) = \int_{\mathbb{R}^3} (\nabla \tilde{\phi})^2 \qquad \text{and} \qquad \int_{\mathbb{R}^3} \tilde{\phi}^2 \leq N.$$

Furthermore, $\tilde{\phi}$ can be chosen in such a way that one has, for all $\delta > 0$,

$$\sum_{k \in \mathbb{Z}^3} \left\langle \hat{n}_0^{(k)} \right\rangle^{5/4} l^{-3/4} \leq (1+\delta) \int_{\mathbb{R}^3} \tilde{\phi}^{5/2} + \delta \int_{\mathbb{R}^3} (\nabla \tilde{\phi})^2 + C\delta^{-7} l^8 N^3 + C\delta^{-3/2} l^{-3/4} (L/l)^3,$$

$$\sum_{k \in \mathbb{Z}^3} \left\langle \hat{n}_0^{(k)} \right\rangle^{5/3} l^{-1/3} \leq C (N^{2/5} l)^{5/3} \int_{\mathbb{R}^3} (\nabla \tilde{\phi})^2 + Cl^{-1/3} (L/l)^3.$$

With these three results the main theorem is proven.

Proof of Theorem 4.1. From Theorems 4.3, 4.4 and 4.5 one has the lower bound for the ground state energy of the polaron system

$$\begin{aligned} E_1^{(b)}(N) &\geq \gamma\tilde{\gamma}\inf\left\{\gamma_{\varepsilon,t}\,T(S_0^{\psi}) + \inf_{\sigma}\sum_{k\in\mathbb{Z}^3}\Big(\psi,\tilde{H}^{(k)}\psi\Big) :\ \psi\in\mathcal{H}_0 \text{ with } \|\psi\| = 1\right\} \\ &\quad - L^3 l^{-5} - Ct^{-4}Nl^{-1} - N^{7/5}\Big(Ct^{-2}(N^{1/5}L)^{-2} + Ct^{-4}(N^{1/5}L)^{-1}N^{-1/5}\Big). \\ &\geq \inf\left\{A\int_{\mathbb{R}^3}|\nabla\tilde{\phi}|^2\,\mathrm{d}x - B\int_{\mathbb{R}^3}|\tilde{\phi}|^{5/2}\,\mathrm{d}x :\ \tilde{\phi}\in H^1(\mathbb{R}^3) \text{ with } \int_{\mathbb{R}^3}|\tilde{\phi}|^2\,\mathrm{d}x \leq N\right\} - DN^{7/5}. \end{aligned}$$

The coefficients are

$$\begin{aligned} A &= \gamma\tilde{\gamma}\gamma_{\varepsilon,t} - \gamma\tilde{\gamma}\gamma_{\varepsilon,t}^{-1/4}I_0\delta - C\varepsilon^{1/6} - CK(\varepsilon,t,N,l) \\ B &= (1+\delta)\gamma\tilde{\gamma}\Big(\gamma_{\varepsilon,t}^{-1/4}I_0 + K(\varepsilon,t,N,l)\Big) \\ D &= Ct^{-2}(N^{1/5}L)^{-2} + Ct^{-4}(N^{1/5}L)^{-1}N^{-1/5} \\ &\quad + C\gamma\tilde{\gamma}\Big(\varepsilon^{-1}t^{-6}(N^{2/5}l)^{-1} + t^{-22}(N^{1/5}L)^3(N^{2/5}l)^{-5} + \varepsilon^{-1}t^{-8}N^{-2/5} \\ &\quad + \Big(\gamma_{\varepsilon,t}^{-1/4}I_0 + K(\varepsilon,t,N,l)\Big)\delta^{-7}(N^{2/5}l)^8 N^{-8/5} \\ &\quad + \Big(\gamma_{\varepsilon,t}^{-1/4}I_0 + K(\varepsilon,t,N,l)\Big)\delta^{-3/2}(N^{1/5}L)^3(N^{2/5}l)^{-15/4}N^{-1/2} \\ &\quad + \Big(\varepsilon^{1/6} + K(\varepsilon,t,N,l)\Big)(N^{1/5}L)^3(N^{2/5}l)^{-10/3}N^{-2/3}\Big). \end{aligned}$$

Here, $K(\varepsilon,t,N,l)$ is a finite sum consisting of terms that have the form $C\varepsilon^{-a}t^{-b}\Big(N^{2/5}l\Big)^{c}N^{-d}$ with $d > 0$. Note that the sum of the local particle numbers is the total particle number, i.e. $\sum_{k\in\mathbb{Z}} n^{(k)} = N$ and the sum over 1 can be estimated

$$\sum_{k,n^{(k)}\neq 0} l^{-2} \leq L^3/l^5 = N^{7/5}(N^{1/5}L)^3(N^{2/5}l)^{-5}.$$

Note that the conditions that are used in Sections 4.2-4.7 are

$$\begin{aligned} C_1 N l^3 \leq \varepsilon^3 &\iff \varepsilon^{-3}(N^{2/5}l)^3 N^{-1/6} \leq C_1^{-1}, \\ C_1 l < \varepsilon t^4 &\iff \varepsilon^{-1}t^{-4}(N^{2/5}l)N^{-2/5} < C_1^{-1}, \\ \varepsilon^{-1/2}l^{3/2} < R &\iff \varepsilon^{-1/2}t^{-4}(N^{2/5}l)^{1/2}N^{-1/5} < C^{-1}, \end{aligned} \tag{4.8}$$

where the last condition ensures that the short distance cutoff r is less than R.

Now it is shown that $\varepsilon, t, \delta, l$ and L can be chosen in such a way that $A \to 1$, $B \to I_0$ and $D \to 0$ as $N \to \infty$ and such that the conditions (4.8) are satisfied, as well.

- First of all, choose $l \propto N^{-2/5+\delta_l}$ for such a small $\delta_l > 0$ that all terms of the form $(N^{2/5}l)^c N^{-d}$ in A, B, D and (4.8) still go to zero as $N \to \infty$.
- Then, choose $L \propto N^{-1/5+\delta_L}$ for such a small $\delta_L > 0$ that $(N^{1/5}L)^3(N^{2/5}l)^{-5}$ still goes to zero as $N \to \infty$ as well as all terms of the form $(N^{1/5}L)^b(N^{2/5}l)^c N^{-d}$.

- Finally, let ε, t, δ tend to zero so slowly that all terms in D and (4.8) as well as all terms in $K(\varepsilon, t, N, l)$ still tend to zero.

Furthermore, one has that $\gamma, \tilde{\gamma}, \gamma_{\varepsilon,t} \to 1$ as $\varepsilon, t \to 0$. To deduce the proposition define the rescaled wave function

$$\phi(z) = (AI_0)^{6/5} B^{-6/5} N^{-8/10} \tilde{\phi}\Big((AI_0)^{4/5} B^{-4/5} N^{-1/5} z\Big),$$

and the new coordinates $z = B^{4/5}(AI_0)^{-4/5} N^{1/5} x$ for $x \in \mathbb{R}^3$. Note that the norm of the rescaled wave function is bounded $\int_{\mathbb{R}^3} |\phi|^2 \,\mathrm{d}z \leq 1$ since $\int_{\mathbb{R}^3} |\tilde{\phi}|^2 \,\mathrm{d}x \leq N$. Therefore, one has the equality

$$A \int_{\mathbb{R}^3} |\boldsymbol{\nabla}_x \tilde{\phi}|^2 \,\mathrm{d}x - B \int_{\mathbb{R}^3} |\tilde{\phi}|^{5/2} \,\mathrm{d}x = A^{-3/5} B^{8/5} I_0^{-8/5} N^{7/5} \Big(\int_{\mathbb{R}^3} |\boldsymbol{\nabla}_z \phi|^2 \,\mathrm{d}z - I_0 \int_{\mathbb{R}^3} |\phi|^{5/2} \,\mathrm{d}z \Big).$$

Since $A \to 1$ and $B \to I_0$ as $N \to \infty$, Theorem 4.1 follows. □

4.2 Short Distance Cutoff and Second Quantization

From this point on up to Section 4.7, $\tilde{H}^{(k)}$ is estimated from below. For this purpose choose one fixed $\sigma \in L^1(\mathbb{R}^3)$ with $D(\sigma, \sigma) < \infty$. Since the lower bound for $\tilde{H}^{(k)}$ will be independent of σ, it also holds for the infimum over all σ.

The local Hamiltonian $\tilde{H}^{(k)}$ and the local particle number $\hat{n}^{(k)}$ commute. Therefore, one can assume ψ to be in an eigenspace of $\hat{n}^{(k)}$ for all $k \in \mathbb{Z}^3$ and work with the eigenvalues $n^{(k)}$ of the operator $\hat{n}^{(k)}$ in the state ψ. Furthermore, the index (k) will be suppressed for the sake of readability. However, the reader should keep in mind that this treatment is done in the small cube $Q_l(kl)$.

It turns out that the energy of a cube is not relevant for the leading order if the particle number n is too small or too big. This is why, for sections 4.2-4.6, it is assumed

$$C_1 \varepsilon \omega(t)^2 \leq nl \leq \varepsilon^{-4} (N^{2/5} l)^{10}. \tag{4.9}$$

The other case is easily estimated as subleading by using Lemma 4.7 (which does not need this assumption on nl). Choose the constant $C_1 > 0$ as in Lemmas 9.1 and 11.2 of [37].

In various places the two-body interaction of the Hamiltonian has to be bounded by its supremum. This is why, in this section, w_R as defined in (4.7) is replaced by

$$w_{r,R}(y, z) = \chi_l(y) V_{r,R}(y - z) \chi_l(z), \tag{4.10}$$

where the regularized potential is defined

$$V_{r,R}(z) = \frac{\mathrm{e}^{-|z|/R} - \mathrm{e}^{-|z|/r}}{|z|}.$$

Here, the cutoffs are introduced

$$r = (nl)^{-1/2} l^{3/2} \qquad \text{and} \qquad R = \eta\, \omega(t)^{-1} l, \tag{4.11}$$

where $\omega(t) = C_\omega t^{-4} \geq 1$ and $\eta = (1 + 2l/L)^{-1} \leq 1$. (Note that a small and unimportant mistake in [37] is corrected by introducing η.) By choosing $l = N^{-2/5+\delta_l}$ for a small $\delta_l > 0$ and by using (4.9), one gets $r \leq \varepsilon^{-1/2} l^{3/2} < R$ for large N, if ε and t tend to 0 sufficiently slowly.

Note that the bounds hold

$$0 \leq w_{r,R}(y,z) \leq \frac{1}{r}, \qquad \text{and} \qquad \sup_{y\in\mathbb{R}^3} \int_{\mathbb{R}^3} w_{r,R}(y,z)\,\mathrm{d}z \leq 4\pi R^2. \tag{4.12}$$

Define the Hamiltonian with a short distance cutoff in the potential

$$\begin{aligned}\tilde{H}_{r,R} = &\sum_{i=1}^{N} \Big(\gamma_{\varepsilon,t}\mathcal{K}_i - \frac{1}{2}\varepsilon\gamma_{\varepsilon,t}\,\Delta_{i,\mathrm{Neu}}\Big) + \sum_{1\leq i<j\leq N} w_{r,R}(x_i,x_j) \\ &- \sum_{i=1}^{N} \int_{\mathbb{R}^3} \sigma(y) w_{r,R}(y,x_i)\,\mathrm{d}y + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \sigma(y) w_{r,R}(y,z)\sigma(z)\,\mathrm{d}y\,\mathrm{d}z\,.\end{aligned}$$

Lemma 4.6 (A lower bound with a regularized potential)**.** *The Hamiltonian on a small cube is bounded from below by*

$$\tilde{H} \geq \tilde{H}_{r,R} - Cn^2\Big(\varepsilon^{-3/2} r^{1/2} + r^2 l^{-3}\Big).$$

To prove this lemma, note that one can bound the Hamiltonian of a one component charged Bose gas with background σ

$$H_w^{(N)} := \sum_{i=1}^{N} T_i + \sum_{1\leq i<j\leq N} w(x_i,x_j) - \sum_{i=1}^{N} \int_{\mathbb{R}^3} \sigma(y) w(y,x_i)\,\mathrm{d}y + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \sigma(y) w(y,z)\sigma(z)\,\mathrm{d}y\,\mathrm{d}z\,,$$

from below by the Hamiltonian of a two component Bose gas [37], with charges $e_i = 1$ for $1 \leq i \leq N$ and $e_i = -1$ for $N+1 \leq i \leq 2N$,

$$\mathcal{H}_w^{(2N)} := \sum_{i=1}^{2N} T_i \; + \sum_{1\leq i<j\leq 2N} e_i e_j w(x_i,x_j),$$

if the interaction $w \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ has a positive Fourier transform. Here, it is assumed that the definition spaces of $H_w^{(N)}$ and $\mathcal{H}_w^{(N)}$ contain $H^1((\mathbb{R}^3)^N)$.

This estimate is used in [3] to prove a lower bound on the energy of the polaron system that is not sharp. It is made precise in the following lemma which will help to transfer results of [37] to this case. Its proof is elementary and left to the reader.

Lemma 4.7. *For a normalized wave function $\psi \in H^1((\mathbb{R}^3)^N)$, we have*

$$\Big(\psi, H_w^{(N)}\psi\Big) \geq \frac{1}{2}\Big(\psi\otimes\psi, \mathcal{H}_w^{(2N)}\psi\otimes\psi\Big), \tag{4.13}$$

where $(\psi\otimes\psi)(x,y) := \psi(x)\psi(y)$ for all $x, y \in (\mathbb{R}^3)^N$.

Note that a different convention is used for the factor of the kinetic energy than [37]. When using Lemma 4.7 to transfer results from [37] to this case one therefore has to rescale them.

Proof of Lemma 4.6. The error term that one gets by introducing a short distance cutoff is estimated by the corresponding error term in the two component Bose gas [37]. To do so, use Lemma 4.7 with $w := w_r$ as defined in (4.7) and $T_i := -\frac{1}{2}\varepsilon\,\Delta_{i,\mathrm{Neu}}$. Then, equation (4.13) yields

$$\Big(\psi, H_{w_r}^{(N)}\psi\Big) \geq \frac{1}{2}\Big(\psi\otimes\psi, \mathcal{H}_{w_r}^{(2N)}\psi\otimes\psi\Big) \geq -Cn^2(\varepsilon^{-3/2}r^{1/2} + r^2 l^{-3}).$$

In the last inequality Lemma 6.1 of [37] is used. The lemma follows since introducing a short distance cutoff means subtracting the potential terms of $H_{w_r}^{(N)}$. □

In order to bound the ground state energy of the Hamiltonian $\tilde{H}_{r,R}$ in the coming sections from below, the second quantization of the Hamiltonian is used (similar to [37]). For this purpose, for $p \in \pi l^{-1}\mathbb{N}_0^3$, define as in [37]

$$u_p(z) = c_p l^{-3/2}\prod_{i=1}^{3}\cos(p_i(z_i + l/2)),$$

for $z \in \mathbb{R}^3$ and with $c_0 = 1$ and $1 \leq c_p \leq C$ for all p. Then, $\{u_p : p \in \pi l^{-1}\mathbb{N}_0^3\}$ is an orthonormal basis consisting of eigenfunctions of the Laplacian $-\Delta_{\mathrm{Neu}}$ with Neumann boundary condition. In particular, the state $u_0 = l^{-3/2}$ is constant.

With the annihilation operators $a_p := a(u_p)$ and creation operators $a_p^* := a^*(u_p)$ one can write the Hamiltonian as

$$\begin{aligned}\tilde{H}_{r,R} = {} & \gamma_{\varepsilon,t}\sum_{i=1}^{N}\Big(\mathcal{K}_i - \frac{1}{2}\varepsilon\,\Delta_{i,\mathrm{Neu}}\Big) + \frac{1}{2}\sum_{pq\mu\nu}\hat{\omega}_{pq\mu\nu}a_p^*a_q^*a_\mu a_\nu \\ & - \sum_{pq\alpha} l^{3/2}\hat{\sigma}_\alpha\,\hat{\omega}_{p\alpha q0}a_p^*a_q + \frac{1}{2}\sum_{\alpha\beta} l^3\hat{\sigma}_\alpha\hat{\sigma}_\beta\,\hat{\omega}_{\alpha\beta 00},\end{aligned} \tag{4.14}$$

where the Fourier coefficients are defined by $\hat{\sigma}_\alpha = \int_{Q_l} u_\alpha(z)\sigma(z)\,\mathrm{d}z$ and

$$\hat{\omega}_{pq\mu\nu} = \int_{Q_l}\int_{Q_l} u_p(y)u_q(z)w_{r,R}(y,z)u_\mu(y)u_\nu(z)\,\mathrm{d}y\,\mathrm{d}z\,.$$

Using $w_{r,R}(y,z) = w_{r,R}(z,y)$, one immediately concludes the symmetry properties

$$\hat{\omega}_{pq\mu\nu} = \hat{\omega}_{\mu qp\nu}, \quad \hat{\omega}_{pq\mu\nu} = \hat{\omega}_{p\nu\mu q} \quad \text{and} \quad \hat{\omega}_{pq\mu\nu} = \hat{\omega}_{qp\nu\mu}. \tag{4.15}$$

Furthermore, the bound $\sup_y \int w_{r,R}(y,z)\,\mathrm{d}z \leq 4\pi R^2$ (stated in (4.12)) implies

$$|\hat{\omega}_{pq\mu\nu}| \leq 4\pi R^2 l^{-3}, \tag{4.16}$$

for all p, q, μ, ν.

4.3 The Leading Order Estimate

This section covers the estimates that contribute to the ground state energy at leading order. It is similar to section 6 in [36] and mainly differs from it in two ways. First of all, the neutrality term is different since it is a function of space in this case and secondly, it is not necessary to bring the kinetic energy into the desired form in this thesis since the corresponding result of [37] can be used.

Define the main part of the Hamiltonian

$$\begin{aligned} H_{\text{main}} &= \sum_{i=1}^{N} \gamma_{\varepsilon,t}\mathcal{K}_i + \frac{1}{2}\sum_{pq\neq 0} \hat{\omega}_{pq,00}\Big(a_p^* a_0^* a_0 a_q + a_0^* a_p^* a_q a_0 + a_p^* a_q^* a_0 a_0 + a_0^* a_0^* a_p a_q\Big) \\ &= \sum_{i=1}^{N} \gamma_{\varepsilon,t}\mathcal{K}_i + \sum_{pq\neq 0} \hat{\omega}_{pq,00}\bigg(a_p^* a_q a_0^* a_0 + \frac{1}{2} a_p^* a_q^* a_0 a_0 + \frac{1}{2} a_0^* a_0^* a_p a_q\bigg). \end{aligned} \tag{4.17}$$

Since one cannot control either of the terms in equation (4.37) of the subleading part well, the following non-neutrality term has to be included in the treatment of the leading order part. This is why the "quadratic" Hamiltonian is defined

$$\begin{aligned} H_{\text{Q}} =& \sum_{i=1}^{N} \gamma_{\varepsilon,t}\mathcal{K}_i + \sum_{pq\neq 0} \hat{\omega}_{pq,00}\bigg(a_p^* a_q a_0^* a_0 + \frac{1}{2} a_p^* a_q^* a_0 a_0 + \frac{1}{2} a_0^* a_0^* a_p a_q\bigg) \\ &+ \sum_{p\neq 0}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} (nl^{-3} - \sigma(y))\, w_{r,R}(y,z)\, u_0 u_p(z)\, a_p^* a_0 \,\mathrm{d}y\,\mathrm{d}z \\ &+ \sum_{p\neq 0}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} u_0 u_p(y)\, a_0^* a_p\, w_{r,R}(y,z)\, (nl^{-3} - \sigma(z))\,\mathrm{d}y\,\mathrm{d}z\,. \end{aligned} \tag{4.18}$$

Bogolubov's idea in [5] was to replace the operators $a_0^\#$ by $\sqrt{N_0}$. So H_{Q} is called like this because it is quadratic in $a_p^\#$ with $p \neq 0$. In this section the Hamiltonian H_{Q} is bounded from below for an arbitrary σ. This will give a lower bound for H_{main}, too, since one can just set $\sigma = nl^{-3}$ to eliminate the term with a single $a_p^\#$, where $p \neq 0$.

Since all of the small cubes inside of the large one are equivalent, one can simply consider the cube $Q_l = (-l/2, l/2)^3$, i.e. set $k = 0$ in this section. Then the following theorem holds.

Theorem 4.8 (The leading order estimate)**.** *Suppose $C_1\varepsilon\omega(t)^2 \leq nl$. Then, for any σ, the quadratic Hamiltonian is bounded below as*

$$H_Q \;\geq\; -\gamma_{\varepsilon,t}^{-1/4} I_0 n^{5/4} l^{-3/4} - \frac{1}{2}\Big\|nl^{-3} - \sigma\Big\|_{r,R}^2 - C\varepsilon^{-1}t^{-22}nl^{-1}, \tag{4.19}$$

where the coefficient I_0 is defined in equation (1.27) *of the introduction and $\|nl^{-3} - \sigma\|_{r,R}^2$ is defined in the beginning of the next section.*

By setting $\sigma = nl^{-3}$, one gets the bound for the main part of the Hamiltonian

$$H_{\text{main}} \;\geq\; -\gamma_{\varepsilon,t}^{-1/4} I_0 n^{5/4} l^{-3/4} - C\varepsilon^{-1}t^{-22}nl^{-1}. \tag{4.20}$$

In order to prove this theorem, some definitions are needed. Similar to [37], let $\chi_{l,k}(z) = \mathrm{e}^{\mathrm{i}kz}\chi_l(z)$ for $z, k \in \mathbb{R}^3$. Furthermore, introduce the operators

$$b_k^* = a^*(\mathcal{P}\chi_{l,k})\, a_0 \quad \text{and} \quad b_k = a(\mathcal{P}\chi_{l,k})\, a_0^*,$$

for $k \in \mathbb{R}^3$. Here, $\mathcal{P}$ is the projection on the subspace of $L^2(Q_l)$ orthogonal to constants. One then has the commutation relations $[b_k, b_{k'}] = [b_k^*, b_{k'}^*] = 0$ and

$$\begin{aligned}[b_k, b_k^*] &= (\mathcal{P}\chi_{l,k}, \mathcal{P}\chi_{l,k})\, a_0^* a_0 - a^*(\mathcal{P}\chi_{l,k}) a(\mathcal{P}\chi_{l,k}) \\ &\leq \int_{\mathbb{R}^3} \chi_l(z)^2 \,\mathrm{d}z\; a_0^* a_0 \;\leq\; l^3 n. \end{aligned} \tag{4.21}$$

The next step is to express H_{Q} in terms of the operators b_k and b_k^*. For this purpose, as in [36] let

$$\begin{aligned} h_{\mathrm{Q}}(k) =& \frac{\gamma_{\varepsilon,t}}{2(2\pi)^3}\, \frac{1}{n+1}\, \frac{|k|^4}{|k|^2 + (lt^6)^{-2}} \Big(b_k^* b_k + b_{-k}^* b_{-k} \Big) \\ &+ \frac{\widehat{V}_{r,R}(k)}{2 l^{3/2}} \Big(\tau(k)(b_k^* + b_{-k}) + \overline{\tau(k)}(b_k + b_{-k}^*) \\ &\qquad + (2\pi l)^{-3/2} \Big(b_k^* b_k + b_{-k}^* b_{-k} + b_k^* b_{-k}^* + b_k b_{-k} \Big) \Big), \end{aligned} \tag{4.22}$$

with the Fourier transform $\tau := \mathfrak{F}[(nl^{-3} - \sigma)\chi_l] = (2\pi)^{-3/2} \int_{\mathbb{R}^3} (nl^{-3} - \sigma(x))\chi_l(x) \mathrm{e}^{-\mathrm{i}x\cdot}\,\mathrm{d}x$.

Lemma 4.9. *One has the lower bound*

$$H_{\mathrm{Q}} \geq \int_{\mathbb{R}^3} h_{\mathrm{Q}}(k)\,\mathrm{d}k - \sum_{pq \neq 0} \hat{\omega}_{pq00}\, a_p^* a_q. \tag{4.23}$$

Proof. First of all, rewrite the kinetic energy as in [37]

$$\begin{aligned} \gamma_{\varepsilon,t} \sum_{i=1}^{N} \mathcal{K}_i &= \gamma_{\varepsilon,t} \sum_{pq} (u_p, \mathcal{K} u_q)\, a_p^* a_q \\ &= \gamma_{\varepsilon,t} (2\pi)^{-3} \int_{\mathbb{R}^3} \frac{|k|^4}{|k|^2 + (lt^6)^{-2}} \sum_{pq \neq 0} (u_p, \chi_{l,k})(\chi_{l,k}, u_q)\, a_p^* a_q \,\mathrm{d}k \\ &= \gamma_{\varepsilon,t} (2\pi)^{-3} \int_{\mathbb{R}^3} \frac{|k|^4}{|k|^2 + (lt^6)^{-2}} a^*(\mathcal{P}\chi_{l,k}) a(\mathcal{P}\chi_{l,k}) \,\mathrm{d}k\,, \end{aligned}$$

where it is used

$$a^*(\mathcal{P}\chi_{k,l}) = \sum_{p \neq 0} (u_p, \chi_{k,l})\, a_p^* \quad \text{and} \quad a(\mathcal{P}\chi_{k,l}) = \sum_{q \neq 0} (\chi_{k,l}, u_q)\, a_q. \tag{4.24}$$

One arrives at the first term of (4.22) by estimating

$$a^*(\mathcal{P}\chi_{l,k}) a(\mathcal{P}\chi_{l,k}) \geq (n+1)^{-1} a^*(\mathcal{P}\chi_{l,k}) a_0 a_0^* a(\mathcal{P}\chi_{l,k}) = (n+1)^{-1} b_k^* b_k.$$

Now turn to the potential. The term with a single $a_p^{\#}$, where $p \neq 0$, is given by

$$\sum_{p\neq 0} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} (nl^{-3} - \sigma(y)) w_{r,R}(y,z) u_0 u_p(z)\, a_p^* a_0 \,\mathrm{d}y\,\mathrm{d}z + \text{ h.c.}$$

To write this term in Fourier space insert

$$w_{r,R}(y,z) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} \widehat{V}_{r,R}(k) \overline{\chi_{l,k}(y)} \chi_{l,k}(z)\,\mathrm{d}k\,,$$

to get the expression

$$(2\pi l)^{-3/2} \int_{\mathbb{R}^3} \Big(\int_{\mathbb{R}^3} (nl^{-3} - \sigma(y)) \overline{\chi_{l,k}(y)}\,\mathrm{d}y \Big) \widehat{V}_{r,R}(k) \sum_{p\neq 0} \Big(\int_{\mathbb{R}^3} u_p(z)\chi_{l,k}(z)\,\mathrm{d}z \Big)\, a_p^* a_0 \,\mathrm{d}k$$
$$+ \text{ h.c.}$$

If one sets $\tau := \mathfrak{F}[(nl^{-3} - \sigma)\chi_l]$ and uses equation (4.24) one arrives at

$$l^{-3/2} \int_{\mathbb{R}^3} \tau(k) \widehat{V}_{r,R}(k)\, b_k^* \,\mathrm{d}k + \text{ h.c.}$$

After symmetrizing, the claim of the lemma is concluded. To do so, note that $V_{r,R}(z) = V_{r,R}(-z)$ and therefore, $\widehat{V}_{r,R}(k) = \widehat{V}_{r,R}(-k)$. Furthermore, since $(nl^{-3} - \sigma)\chi_l$ is real, one has $\tau(-k) = \overline{\tau(k)}$.

The last line of equation (4.22) follows similarly and gives rise to the error term in equation (4.23). □

At this point, one can derive a lower bound on $h_Q(k)$ using a simple version of Bogolubov's argument. For this reason, quote Theorem 6.3 from [36].

Theorem 4.10. *Let $A \geq B > 0$ and $\kappa \in \mathbb{C}$. Then, one has the inequality*

$$\begin{aligned} &A(b_k^* b_k + b_{-k}^* b_{-k}) + B(b_k^* b_{-k}^* + b_k b_{-k}) + \kappa(b_k^* + b_{-k}) + \overline{\kappa}(b_k + b_{-k}^*) \\ &\quad \geq -\frac{1}{2}\Big(A - \sqrt{A^2 - B^2}\Big)\Big([b_k, b_k^*] + \big[b_{-k}, b_{-k}^*\big]\Big) - \frac{2|\kappa|^2}{A+B}. \end{aligned}$$

With the help of this theorem, the main theorem of this section can finally be proven.

Proof of Theorem 4.8. To prove this theorem, first apply Theorem 4.10 to the Hamiltonian h_{Q} defined in equation (4.22). Then, one can progress similar to the proof of Lemma 8.3 in [37] to bring the leading order term into the desired form.

Define the numbers

$$B_k = \frac{\widehat{V}_{r,R}(k)}{2(2\pi)^{3/2} l^3}, \qquad A_k = B_k + \frac{\gamma_{\varepsilon,t}}{2(2\pi)^3} \frac{1}{n+1} \frac{|k|^4}{|k|^2 + (lt^6)^{-2}} \quad \text{and} \quad \kappa_k = \frac{\widehat{V}_{r,R}(k)}{2l^{3/2}} \tau(k).$$

With Theorem 4.10 and equation (4.21) the inequality holds

$$\int_{\mathbb{R}^3} h_{\mathrm{Q}}(k)\,\mathrm{d}k \geq -\int_{\mathbb{R}^3}\Big(A_k - \sqrt{A_k^2 - B_k^2}\Big) n l^3 \,\mathrm{d}k \; - \int_{\mathbb{R}^3} \frac{2|\kappa_k|^2}{A_k + B_k}\,\mathrm{d}k\,. \tag{4.25}$$

Then, use $B_k \leq A_k$ to bound the last integral

$$\int_{\mathbb{R}^3} \frac{2|\kappa_k|^2}{A_k + B_k}\,\mathrm{d}k \leq \int_{\mathbb{R}^3} \frac{|\kappa_k|^2}{B_k}\,\mathrm{d}k = \frac{1}{2}\,(2\pi)^{3/2}\!\int_{\mathbb{R}^3} \widehat{V}_{r,R}(k)|\tau(k)|^2\,\mathrm{d}k = \frac{1}{2}\Big\|nl^{-3} - \sigma\Big\|_{r,R}^2.$$

Thus, one gets the desired neutrality term of (4.19).

Consider the first integral of the lower bound in (4.25). Integrating over αk instead of k with $\alpha = \gamma_{\varepsilon,t}^{-1/4}(n+1)^{1/4} l^{-3/4}$, one gets the integrand

$$\frac{n(n+1)^{1/4} l^{-3/4}}{2(2\pi)^3 \gamma_{\varepsilon,t}^{1/4}}\Big(g(k) + f(k) - \Big((g(k)+f(k))^2 - g(k)^2\Big)^{1/2}\Big), \tag{4.26}$$

where

$$g(k) = 4\pi\bigg(\frac{1}{|k|^2 + (\alpha R)^{-2}} - \frac{1}{|k|^2 + (\alpha r)^{-2}}\bigg) \quad \text{and} \quad f(k) = \frac{|k|^4}{|k|^2 + (\alpha l t^6)^{-2}}.$$

The expression (4.26) is monotone increasing in g. Thus, one can simply estimate $g(k)$ from above by $4\pi|k|^{-2}$. In f it is monotone decreasing. So $f(k)$ has to be bounded from below appropriately. Defining $a = (\alpha l t^6)^{-2} = \gamma_{\varepsilon,t}^{1/2}((n+1)l)^{-1/2} t^{-12}$, estimate

$$\begin{aligned} f(k) &\geq 0, && \text{if } |k|^2 \leq 4a, \\ f(k) &\geq |k|^2 - a, && \text{if } |k|^2 > 4a. \end{aligned}$$

Turning to the root in (4.26) and supposing $|k|^2 > 4a$, estimate

$$\begin{aligned} \Big(\Big(4\pi|k|^{-2} + |k|^2 - a\Big)^2 - (4\pi)^2|k|^{-4}\Big)^{1/2} &\geq \Big(|k|^4 + 8\pi\Big)^{1/2}\bigg(1 - 2a|k|^{-2} + \frac{a^2}{|k|^4 + 8\pi}\bigg)^{1/2} \\ \geq \Big(|k|^4 + 8\pi\Big)^{1/2}\bigg(1 - a|k|^{-2} + \frac{a^2}{2(|k|^4 + 8\pi)} - \frac{1}{2}a^2|k|^{-4} - Ca^3|k|^{-6}\bigg), \end{aligned} \tag{4.27}$$

where the root is expanded about 1 and it is used $a^2(|k|^4 + 8\pi)^{-1} \leq a^2|k|^{-4} \leq 2a|k|^{-2} < 1/2$. Then, (4.27) is bounded from below by

$$\begin{aligned} &\Big(|k|^4 + 8\pi\Big)^{1/2} - a - 8\pi a|k|^{-4} - 4\pi a^2|k|^{-6} - Ca^3|k|^{-4} - Ca^3|k|^{-8} \\ &\geq \Big(|k|^4 + 8\pi\Big)^{1/2} - a - C\varepsilon^{-1}t^{-16}a|k|^{-4}. \end{aligned}$$

Here, the fact is used that $a^2 \le C(nl)^{-1}t^{-24} \le C\varepsilon^{-1}t^{-16}$ since $nl \ge C_1\varepsilon\omega(t)^2$. One therefore gets

$$\begin{aligned}
&\int_{\mathbb{R}^3} \Big(A_k - \sqrt{A_k^2 - B_k^2}\Big) nl^3 \,\mathrm{d}k \\
&\le \frac{n(n+1)^{1/4} l^{-3/4}}{2(2\pi)^3 \gamma_{\varepsilon,t}^{1/4}} \left(\int\limits_{|k|<(4a)^{1/2}} 4\pi|k|^{-2}\,\mathrm{d}k + \int\limits_{|k|>(4a)^{1/2}} \Big(4\pi|k|^{-2} + |k|^2 - \Big(|k|^4 + 8\pi\Big)^{1/2}\Big)\,\mathrm{d}k \right) \\
&\quad + C\varepsilon^{-1}t^{-16} \int\limits_{|k|>(4a)^{1/2}} a|k|^{-4}\,\mathrm{d}k\,.
\end{aligned}$$

Since the error of combining the first two integrals is less then $\int_{|k|<(4a)^{1/2}}(8\pi)^{1/2}\,\mathrm{d}k = Ca^{3/2}$, one gets the upper bound

$$\begin{aligned}
&\frac{n\Big(n^{1/4}+1\Big)l^{-3/4}}{2(2\pi)^3\gamma_{\varepsilon,t}^{1/4}} \left(\int_{\mathbb{R}^3} \Big(4\pi|k|^{-2} + |k|^2 - \Big(|k|^4+8\pi\Big)^{1/2}\Big)\,\mathrm{d}k + C\varepsilon^{-1}t^{-16}a^{1/2} \right) \\
&\le \gamma_{\varepsilon,t}^{-1/4} n^{5/4} l^{-3/4} \frac{2^{1/2}}{\pi^{3/4}} \int_0^\infty \Big(1 + x^4 - x^2(x^4+2)^{1/2}\Big)\,\mathrm{d}x + C\varepsilon^{-1}t^{-22}nl^{-1}.
\end{aligned}$$

The theorem follows by equations (4.23) and (4.30), since

$$\frac{2^{1/2}}{\pi^{3/4}} \int_0^\infty \Big(1 + x^4 - x^2(x^4+2)^{1/2}\Big)\,\mathrm{d}x = \frac{2}{5}\left(\frac{2}{\pi}\right)^{1/4} \frac{\Gamma(3/4)}{\Gamma(5/4)} = I_0.$$

□

4.4 Estimates on the Subleading Terms

This section is concerned with estimating those terms in the Hamiltonian $\tilde{H}_{r,R}$ that do not contribute to the ground state energy at leading order.

These bounds will first be used to prove a-priori bounds in Section 4.5 and then, to prove the lower bound on the Hamiltonian $\tilde{H}$ in Section 4.7. Since different terms are difficult in these two applications, two different lower bounds are proven. The first one that is used to prove the a-priori bounds and the second one to prove the lower bound on $\tilde{H}$.

As in Section 4.3 simply the cube $Q_l = (-l/2, l/2)^3$ is considered in this section.

One can proceed similar to section 5 of [36]. In this case, however, neutrality cannot be expected to hold uniformly in space as the background charge density σ is not constant but depends on the position in space. Therefore, it can only be controlled in the local Coulomb norm

$$\Big\|nl^{-3} - \sigma\Big\|_{r,R} = \left(\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \Big(nl^{-3} - \sigma(y)\Big) w_{r,R}(y,z) \Big(nl^{-3} - \sigma(z)\Big)\,\mathrm{d}y\,\mathrm{d}z \right)^{1/2},$$

where $w_{r,R}$ is defined in equation (4.10). The fact that $\|\cdot\|_{r,R}$ defines a norm follows from $V_{r,R}$ having a positive Fourier transform. This implies that $w_{r,R}$ defines the kernel of a positive integral operator. Using this norm, all of the terms containing σ will be bounded. Then, the following result is deduced.

Theorem 4.11 (Lower bound on the subleading part of the Hamiltonian)**.** *The operator inequality holds*

$$\begin{aligned}\tilde{H}_{r,R} - H_{\mathrm{main}} \geq\ & \frac{1}{2}(1-3\varepsilon')\left\|nl^{-3}-\sigma\right\|_{r,R}^2 + \frac{1}{2}(1-2\varepsilon')\sum_{pq\mu\nu\neq 0}\hat{\omega}_{pq\mu\nu}\, a_p^* a_q^* a_\mu a_\nu \\ & - \Big(1+\frac{1}{2\varepsilon'}\Big)4\pi R^2 l^{-3}\hat{n}_+^2 - \Big(5+\frac{2}{\varepsilon'}\Big)4\pi R^2 l^{-3} n(\hat{n}_+ + 1) \\ & - \sqrt{2}\left\|nl^{-3}-\sigma\right\|_{r,R} r^{-1/2}\hat{n}_+ - \varepsilon' r^{-1}\hat{n}_+. \end{aligned} \tag{4.28}$$

Moreover,

$$\begin{aligned}\tilde{H}_{r,R} - H_{\mathrm{Q}} \geq\ & \frac{1}{2}(1-3\varepsilon')\left\|nl^{-3}-\sigma\right\|_{r,R}^2 + \Big(\frac{1}{2}-\frac{1}{\varepsilon'}\Big)\sum_{pq\mu\nu\neq 0}\hat{\omega}_{pq\mu\nu}\, a_p^* a_q^* a_\mu a_\nu \\ & - \Big(1+\frac{3}{2\varepsilon'}\Big)4\pi R^2 l^{-3}\hat{n}_+^2 - \varepsilon' 12\pi R^2 l^{-3} n\hat{n}_+ - 2\pi R^2 l^{-3} n \\ & - \frac{1}{\varepsilon'}4\pi R^2 l^{-3}(2\hat{n}_+ + 1) - \frac{1}{\varepsilon'} r^{-1}\hat{n}_+(\hat{n}_+ + 1). \end{aligned} \tag{4.29}$$

Proof. Simply combine all estimates of this section in one inequality, i.e. combine Lemma 4.14, 4.15, 4.17 and 4.18. For the first bound, set $\varepsilon'' := \varepsilon'^{-1}$ in Lemma 4.14 and use equation (4.32) in Lemma 4.15 and equation (4.37) in Lemma 4.17. For the second bound, set $\varepsilon'' := \varepsilon'$ in Lemma 4.14 and use equation (4.33) in Lemma 4.15 and equation (4.38) in Lemma 4.17. □

The terms of the Hamiltonian $\tilde{H}_{r,R}$ in (4.14) that shall be treated in this section are the following.

$\hat{\omega}_{pq\mu\nu}$ The terms in the Hamiltonian containing $\omega_{pq\mu\nu}$ with $p, q, \mu, \nu \neq 0$ describe the Coulomb repulsion on functions orthogonal to constants and are thus positive. However, since these terms are needed to bound negative ones, one has to find an upper bound for them.

$\hat{\omega}_{pq\mu 0}$ The terms with coefficients $\omega_{pq\mu 0}$, $\omega_{pq0\nu}$, $\omega_{p0\mu\nu}$ and $\omega_{0q\mu\nu}$ with $p, q, \mu, \nu \neq 0$ are bounded from below in [36]. Therefore, the corresponding the result can be used.

$\hat{\omega}_{p0q0}$ Bounding the terms in the Hamiltonian with $\hat{\omega}_{p0q0}$, $\hat{\omega}_{0p0q}$ or $\hat{\sigma}_\alpha\hat{\omega}_{p\alpha q0}$, where $p, q \neq 0$, from below causes some difficulties since the estimate should contain the neutrality term $\|nl^{-3}-\sigma\|_{r,R}$ without rendering the remainder uncontrollable. To resolve these difficulties a Cauchy-Schwarz operator inequality is proven in Lemma 4.16.

$\hat{\omega}_{p000}$ The terms with coefficients $\hat{\omega}_{p000}$ (or any other permutation of these indices) or $\hat{\sigma}_\alpha \hat{\omega}_{p\alpha 00}$, where $p \neq 0$, form the other most difficult part of the Hamiltonian. They can only be estimated by two terms that cannot be controlled well. This is why one has to take the part containing $nl^{-3} - \sigma$ into the treatment of the leading order part.

$\hat{\omega}_{0000}$ The sum of the terms with $\hat{\omega}_{0000}$, $\hat{\sigma}_\alpha \hat{\omega}_{0\alpha 00}$ or $\hat{\sigma}_\alpha \hat{\sigma}_\beta \hat{\omega}_{\alpha\beta 00}$ as coefficients is basically positive. It will be bounded from below by $\|nl^{-3} - \sigma\|^2_{r,R}$ minus some error.

Quote the following result that is proven in [36].

Lemma 4.12. *One has the operator inequalities*

$$0 \leq \sum_{p,q \neq 0} \hat{\omega}_{pq00}\, a_p^* a_q = \sum_{p,q \neq 0} \hat{\omega}_{p00q}\, a_p^* a_q \leq 4\pi R^2 l^{-3} \hat{n}_+, \tag{4.30}$$

and

$$0 \leq \sum_{p,q,m \neq 0} \hat{\omega}_{pmmq}\, a_p^* a_q \leq r^{-1} \hat{n}_+. \tag{4.31}$$

Proof. See Lemma 5.4 in [36]. □

Then, consider the different parts of the Hamiltonian.

Lemma 4.13 (Bound on terms with $\hat{\omega}_{pq\mu\nu}$)**.** *The following operator inequality holds.*

$$0 \leq \sum_{pq\mu\nu \neq 0} \hat{\omega}_{pq\mu\nu}\, a_p^* a_q^* a_\mu a_\nu \leq r^{-1} \hat{n}_+^2.$$

Proof. The operator $\frac{1}{2}\sum_{pq\mu\nu \neq 0} \hat{\omega}_{pq\mu\nu}\, a_p^* a_q^* a_\mu a_\nu$ is the second quantization of the two-body multiplication operator $(\mathcal{P} \otimes \mathcal{P}) w_{r,R} (\mathcal{P} \otimes \mathcal{P})$. Here, $\mathcal{P}$ denotes the projection onto the functions orthogonal to constants in $L^2(Q_l)$. By equation (4.12) one has for all $y, z \in \mathbb{R}^3$

$$0 \leq w_{r,R}(y,z) \leq \frac{1}{r}.$$

Since the second quantization of of the two-body operator $\mathcal{P} \otimes \mathcal{P}$ is $\frac{1}{2}\hat{n}_+(\hat{n}_+ - 1)$, the lemma follows. □

Lemma 4.14 (Bound on terms with $\hat{\omega}_{pq\mu 0}$)**.** *The sum of all terms in the Hamiltonian with coefficients $\hat{\omega}_{pq\mu 0}$, $\hat{\omega}_{pq0\nu}$, $\hat{\omega}_{p0\mu\nu}$ and $\hat{\omega}_{0q\mu\nu}$, where $p, q, \mu, \nu \neq 0$, has the lower bound*

$$-\varepsilon'' 4\pi R^2 l^{-3} n \hat{n}_+ - \frac{1}{\varepsilon''} r^{-1} \hat{n}_+ - \frac{1}{\varepsilon''} \sum_{pq\mu\nu \neq 0} \hat{\omega}_{pq\mu\nu}\, a_p^* a_q^* a_\mu a_\nu,$$

for all $\varepsilon'' > 0$.

Proof. See Lemma 5.6 of [36]. □

Lemma 4.15 (Bound on terms with $\hat\omega_{p0q0}$)**.** *The sum of all terms in the Hamiltonian with coefficients $\hat\omega_{p0q0}$, $\hat\omega_{0p0q}$ or $\hat\sigma_\alpha\hat\omega_{p\alpha q0}$, where $p, q \neq 0$, has the lower bound*

$$-\sqrt{2}\Big\|nl^{-3} - \sigma\Big\|_{r,R} r^{-1/2}\hat n_+ \;-\; 4\pi R^2 l^{-3}\hat n_+^2. \tag{4.32}$$

Therefore, they are also bounded from below by

$$-\,\varepsilon'\Big\|nl^{-3} - \sigma\Big\|_{r,R}^2 - \frac{1}{2\varepsilon'}\,r^{-1}\hat n_+^2 \;-\; 4\pi R^2 l^{-3}\hat n_+^2, \tag{4.33}$$

for all $\varepsilon' > 0$.

Proof. The symmetry properties (4.15) imply $\hat\omega_{p0q0} = \hat\omega_{0p0q}$. Therefore, the relevant terms are

$$\begin{aligned}
&\sum_{p,q\neq 0}\left(\frac{1}{2}\,\hat\omega_{p0q0}\,a_p^* a_0^* a_q a_0 + \frac{1}{2}\,\hat\omega_{0p0q}\,a_0^* a_p^* a_q a_0 - l^{3/2}\sum_\alpha \hat\sigma_\alpha\,\hat\omega_{p\alpha q0}\,a_p^* a_q\right)\\
&\quad= \sum_{p,q\neq 0}\left(\hat\omega_{p0q0}\hat n_0 - l^{3/2}\sum_\alpha \hat\sigma_\alpha\,\hat\omega_{p\alpha q0}\right) a_p^* a_q\\
&\quad= \sum_{p,q\neq 0}\left(\hat\omega_{p0q0} n - l^{3/2}\sum_\alpha \hat\sigma_\alpha\,\hat\omega_{p\alpha q0}\right) a_p^* a_q - \hat n_+ \sum_{p,q\neq 0}\hat\omega_{p0q0}\,a_p^* a_q.
\end{aligned} \tag{4.34}$$

The second term can be controlled by estimating

$$\begin{aligned}
\hat n_+ \sum_{p,q\neq 0}\hat\omega_{p0q0}\,a_p^* a_q &= l^{-3}\,\hat n_+ \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} w_{r,R}(y,z)\,\mathrm{d}y \left(\sum_{p\neq 0} u_p(z) a_p\right)^{\!*}\left(\sum_{q\neq 0} u_q(z) a_q\right)\mathrm{d}z\\
&\le l^{-3}\,\hat n_+ \sup_{z'}\int_{\mathbb{R}^3} w_{r,R}(y,z')\,\mathrm{d}y \int_{\mathbb{R}^3}\left(\sum_{p,q\neq 0} u_p(z) u_q(z)\,a_p^* a_q\right)\mathrm{d}z \;\le\; 4\pi R^2 l^{-3}\hat n_+^2.
\end{aligned}$$

The last inequality follows from the bound (4.12).

The first term in (4.34) equals

$$\begin{aligned}
&\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\sum_{p,q\neq 0} a_p^* a_q u_p(y) u_q(y) w_{r,R}(y,z)\Big(nl^{-3} - \sigma(z)\Big)\,\mathrm{d}y\,\mathrm{d}z\\
&\ge -\left(\sum_{pq\mu\nu\neq 0}\hat\omega_{p\mu q\nu}\,a_p^* a_q\,a_\mu^* a_\nu\right)^{1/2}\Big\|nl^{-3} - \sigma\Big\|_{r,R}
\end{aligned}$$

where the operator inequality (4.35) of Lemma 4.16 is used. By Lemma 4.13, Lemma 4.12 and the fact that the root is operator monotone, conclude

$$
\begin{aligned}
&- \left\| nl^{-3} - \sigma \right\|_{r,R} \Bigg(\sum_{pq\mu\nu \neq 0} \hat{\omega}_{p\mu q\nu}\, a_p^* a_q\, a_\mu^* a_\nu \Bigg)^{1/2} \\
&= - \left\| nl^{-3} - \sigma \right\|_{r,R} \Bigg(\sum_{pq\mu\nu \neq 0} \hat{\omega}_{p\mu q\nu}\, a_p^* a_\mu^*\, a_q a_\nu \;+ \sum_{pm\nu \neq 0} \hat{\omega}_{pmm\nu}\, a_p^* a_\nu \Bigg)^{1/2} \\
&\geq - \left\| nl^{-3} - \sigma \right\|_{r,R} \left(r^{-1}\hat{n}_+^2 + r^{-1}\hat{n}_+ \right)^{1/2} \;\geq\; - \left\| nl^{-3} - \sigma \right\|_{r,R} \sqrt{2}\, r^{-1/2} \hat{n}_+ .
\end{aligned}
$$

□

To show the missing ingredient of the last proof, let $X \subseteq \mathbb{R}^d$ for some $d \in \mathbb{N}$ and let $W \colon X \times X \to \mathbb{R}$ be symmetric and positive definite. By this it is meant

$$
\forall f \colon X \to \mathbb{C} \colon \quad \int_X \int_X \overline{f(x)} W(x,y) f(y)\, \mathrm{d}x\, \mathrm{d}y \geq 0 .
$$

Furthermore, let $A(x)$ and $B(x)$ be closed and densely defined operators on some separable Hilbert space $\mathcal{H}$ for every $x \in X$. Then, one can state following lemma.

Lemma 4.16 (Operator inequality of Cauchy-Schwarz type). *The following operator inequalities hold. First of all, for the product of a function and an operator*

$$
\begin{aligned}
&\left| \operatorname{Re} \iint_{X\times X} \overline{f(x)} W(x,y) A(y)\, \mathrm{d}x\, \mathrm{d}y \right| \\
&\leq \Bigg(\iint_{X\times X} \overline{f(x)} W(x,y) f(y)\, \mathrm{d}x\, \mathrm{d}y \Bigg)^{1/2} \Bigg(\iint_{X\times X} \frac{1}{2}\Big(A(x)^* A(y) + A(x) A(y)^* \Big) W(x,y)\, \mathrm{d}x\, \mathrm{d}y \Bigg)^{1/2} .
\end{aligned} \tag{4.35}
$$

And secondly, for the product of two operators

$$
\begin{aligned}
&\iint_{X\times X} \Big(A(x)^* B(y) + B(x)^* A(y) \Big) W(x,y)\, \mathrm{d}x\, \mathrm{d}y \\
&\quad \leq \iint_{X\times X} A(x)^* W(x,y) A(y)\, \mathrm{d}x\, \mathrm{d}y + \iint_{X\times X} B(x)^* W(x,y) B(y)\, \mathrm{d}x\, \mathrm{d}y .
\end{aligned} \tag{4.36}
$$

Proof. The second inequality follows from the fact that for all $\phi \in \mathcal{H}$

$$
\Big(\phi, \iint A(x)^* W(x,y) A(y)\, \mathrm{d}x\, \mathrm{d}y\; \phi \Big) = \sum_i \iint (\phi, A(x)^* v_i) W(x,y) (v_i, A(y)\phi)\, \mathrm{d}x\, \mathrm{d}y \geq 0,
$$

for some orthonormal basis $\{v_i\}$ of the separable Hilbert space $\mathcal{H}$.

The first inequality is proven exactly as the Cauchy-Schwarz inequality of a scalar product is proven. For this purpose, define

$$B = \operatorname{Re} \iint \overline{f(x)} W(x,y) A(y)\,\mathrm{d}x\,\mathrm{d}y\,, \qquad \text{and} \qquad [f]_W = \Big(\iint \overline{f(x)} W(x,y) f(y)\,\mathrm{d}x\,\mathrm{d}y\Big)^{1/2}.$$

Then, one gets

$$\begin{aligned} 0 \le & \iint \Big(A(x) - f(x)[f]_W^{-2}\operatorname{Re} B\Big)^* W(x,y)\Big(A(y) - f(y)[f]_W^{-2}\operatorname{Re} B\Big)\,\mathrm{d}x\,\mathrm{d}y \\ & + \iint \Big(A(x) - f(x)[f]_W^{-2}\operatorname{Re} B\Big) W(x,y)\Big(A(y) - f(y)[f]_W^{-2}\operatorname{Re} B\Big)^*\,\mathrm{d}x\,\mathrm{d}y \\ & = \iint \Big(A(x)^*A(y) + A(x)A(y)^*\Big) W(x,y)\,\mathrm{d}x\,\mathrm{d}y \;+\; 2[f]_W^{-2}(\operatorname{Re} B)^2 \\ & - \Big(\iint A(x)^* W(x,y) f(y)\,\mathrm{d}x\,\mathrm{d}y + \iint A(x) W(x,y)\overline{f(y)}\,\mathrm{d}x\,\mathrm{d}y\Big)\,(\operatorname{Re} B)[f]_W^{-2} \\ & - (\operatorname{Re} B)[f]_W^{-2}\Big(\iint \overline{f(x)} W(x,y) A(y)\,\mathrm{d}x\,\mathrm{d}y + \iint f(x) W(x,y) A(y)^*\,\mathrm{d}x\,\mathrm{d}y\Big) \\ & = \iint \Big(A(x)^*A(y) + A(x)A(y)^*\Big) W(x,y)\,\mathrm{d}x\,\mathrm{d}y \;-\; 2[f]_W^{-2}(\operatorname{Re} B)^2. \end{aligned}$$

This is equivalent to the inequality

$$\Big(\operatorname{Re} \iint \overline{f(x)} W(x,y) A(y)\,\mathrm{d}x\,\mathrm{d}y\Big)^2 \le [f]_W^2 \iint \frac{1}{2}\Big(A(x)^*A(y) + A(x)A(y)^*\Big) W(x,y)\,\mathrm{d}x\,\mathrm{d}y\,.$$

The lemma follows since the root is operator monotone. □

Lemma 4.17 (Bound on terms with $\hat\omega_{p000}$)**.** *The sum of all terms in the Hamiltonian with coefficients $\hat\omega_{p000}$ (or any other permutation of these indices) or $\hat\sigma_\alpha\hat\omega_{p\alpha00}$, where $p \neq 0$, has the lower bound*

$$-\varepsilon'\Big\|nl^{-3} - \sigma\Big\|_{r,R}^2 - \Big(\frac{2}{\varepsilon'} + 4\Big) 4\pi R^2 l^{-3} n(\hat n_+ + 1), \tag{4.37}$$

for all $\varepsilon' > 0$, or alternatively,

$$\begin{aligned} \sum_{p\neq 0} \int_{\mathbb{R}^3}\!\int_{\mathbb{R}^3} \Big(u_0 u_p(y)\, a_p^* a_0\, w_{r,R}(y,z)(nl^{-3} - \sigma(z)) + (nl^{-3} - \sigma(y))\, w_{r,R}(y,z) u_0 u_p(z)\, a_0^* a_p\Big)\,\mathrm{d}y\,\mathrm{d}z \\ -\varepsilon' 8\pi R^2 l^{-3} n \hat n_+ - \frac{1}{\varepsilon'} 4\pi R^2 l^{-3}(\hat n_+ + 1)^2, \end{aligned} \tag{4.38}$$

for all $\varepsilon' > 0$.

Proof. The relevant terms are

$$\frac{1}{2}\sum_{p\neq 0}\Big(\hat{\omega}_{p000}\big(2a_p^*a_0^*a_0a_0+2a_0^*a_0^*a_0a_p\big)-2l^{3/2}\sum_{\alpha}\hat{\sigma}_\alpha\hat{\omega}_{p\alpha 00}\big(a_p^*a_0+a_0^*a_p\big)\Big)$$

$$=\sum_{p\neq 0}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\Big((\hat{n}_0l^{-3}-\sigma(y))w_{r,R}(y,z)u_0u_p(z)\,a_p^*a_0$$

$$+u_0u_p(y)\,a_0^*a_pw_{r,R}(y,z)(\hat{n}_0l^{-3}-\sigma(z))\Big)\,\mathrm{d}y\,\mathrm{d}z$$

$$=\sum_{p\neq 0}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\Big(u_0u_p(z)\,a_p^*a_0w_{r,R}(y,z)((\hat{n}_0-1)l^{-3}-\sigma(y))$$

$$+((\hat{n}_0-1)l^{-3}-\sigma(z))w_{r,R}(y,z)u_0u_p(y)\,a_0^*a_p\Big)\,\mathrm{d}y\,\mathrm{d}z$$

If we now insert $\hat{n}_0=n-\hat{n}_+$, we arrive at

$$\sum_{p\neq 0}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\Big(u_0u_p(z)\,a_p^*a_0\,w_{r,R}(z,y)(nl^{-3}-\sigma(y))+(nl^{-3}-\sigma(z))\,w_{r,R}(z,y)u_0u_p(y)\,a_0^*a_p\Big)\,\mathrm{d}y\,\mathrm{d}z$$
$$+\sum_{p\neq 0}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\Big(u_0u_p(z)\,a_p^*a_0\,w_{r,R}(z,y)(\hat{n}_++1)l^{-3}+(\hat{n}_++1)l^{-3}\,w_{r,R}(z,y)u_0u_p(y)\,a_0^*a_p\Big)\,\mathrm{d}y\,\mathrm{d}z \tag{4.39}$$

The first sum in (4.39) is already the desired first term of the alternative bound (4.38). Since $w_{r,R}$ defines a positive integral operator, one has the Cauchy Schwarz inequality (4.36) and thus, the second sum in (4.39) is bounded below by

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\Bigg(\varepsilon'\sum_{p,q\neq 0}u_0u_p(z)\,a_p^*a_0w_{r,R}(z,y)u_0u_q(y)\,a_qa_0^*$$
$$+\frac{1}{\varepsilon'}(\hat{n}_++1)l^{-3}w_{r,R}(z,y)(\hat{n}_++1)l^{-3}\Bigg)\,\mathrm{d}y\,\mathrm{d}z$$
$$\geq -\varepsilon'(\hat{n}_0+1)\sum_{p,q\neq 0}\hat{\omega}_{pq00}\,a_p^*a_q-\frac{1}{\varepsilon'}\hat{\omega}_{0000}(\hat{n}_++1)^2$$
$$\geq -\varepsilon' 8\pi R^2l^{-3}n\hat{n}_+-\frac{1}{\varepsilon'}4\pi R^2l^{-3}(\hat{n}_++1)^2. \tag{4.40}$$

Here, the commutator relation $[a_0,a_0^*]=1$ and equation (4.30) from Lemma 4.12 are used. Furthermore, it is assumed $n+1\leq 2n$. This concludes the proof of the alternative bound (4.38).

Now turn to the proof of the first bound (4.37). Use equation (4.40) with $\varepsilon'=1$ to bound the second term in (4.39) from below by

$$-4\pi R^2l^{-3}2n\hat{n}_+-4\pi R^2l^{-3}2n(\hat{n}_++1)\;\geq\;-4\cdot 4\pi R^2l^{-3}n(\hat{n}_++1),$$

assuming $n+1 \leq 2n$. Finally, the lemma follows by estimating the first term in (4.39) with the help of the Cauchy-Schwarz inequality (4.36)

$$\begin{aligned}
&\sum_{p\neq 0} \iint_{\mathbb{R}^3\mathbb{R}^3} \Big(u_0 u_p(z)\, a_p^* a_0\, w_{r,R}(z,y)(nl^{-3} - \sigma(y)) + (nl^{-3} - \sigma(z))\, w_{r,R}(z,y) u_0 u_p(y)\, a_0^* a_p \Big)\, \mathrm{d}y\, \mathrm{d}z \\
&\geq -\varepsilon' \Big\| \sigma - nl^{-3} \Big\|_{r,R}^2 - \frac{1}{\varepsilon'} \iint_{\mathbb{R}^3\mathbb{R}^3} \sum_{p,q\neq 0} u_0 u_p(z)\, a_p^* a_0 w_{r,R}(z,y) u_0 u_q(y)\, a_q a_0^*\, \mathrm{d}y\, \mathrm{d}z \\
&= -\varepsilon' \Big\| \sigma - nl^{-3} \Big\|_{r,R}^2 - \frac{1}{\varepsilon'} \sum_{p,q\neq 0} \hat{\omega}_{pq00}\, a_p^* a_q (\hat{n}_0 + 1) \\
&\geq -\varepsilon' \Big\| \sigma - \hat{n}_0 l^{-3} \Big\|_{r,R}^2 - \frac{1}{\varepsilon'} 8\pi R^2 l^{-3} n \hat{n}_+,
\end{aligned}$$

where equation (4.30) of Lemma 4.12 is used to bound the second term from below. □

Lemma 4.18 (Bound on terms with $\hat{\omega}_{0000}$)**.** *The terms with coefficients $\hat{\omega}_{0000}$, $\hat{\sigma}_\alpha \hat{\omega}_{\alpha 000}$ or $\hat{\sigma}_\alpha \hat{\sigma}_\beta \hat{\omega}_{\alpha\beta 00}$ are bounded below by*

$$\frac{1}{2}(1-\varepsilon') \Big\| nl^{-3} - \sigma \Big\|_{r,R}^2 - \frac{1}{\varepsilon'} 2\pi R^2 l^{-3} \hat{n}_+^2 - 2\pi R^2 l^{-3} n. \tag{4.41}$$

Proof. The relevant terms are

$$\begin{aligned}
&\frac{1}{2}\, \hat{\omega}_{0000}\, a_0^* a_0^* a_0 a_0 - l^{3/2} \sum_\alpha \hat{\sigma}_\alpha\, \hat{\omega}_{\alpha 000}\, a_0^* a_0 + \frac{1}{2} l^3 \sum_{\alpha,\beta} \hat{\sigma}_\alpha \hat{\sigma}_\beta\, \hat{\omega}_{\alpha\beta 00} \\
&= \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \Big(\hat{n}_0 l^{-3}\, w_{r,R}(y,z)\, \hat{n}_0 l^{-3} - 2\sigma(y)\, w_{r,R}(y,z)\, \hat{n}_0 l^{-3} + \sigma(y)\, w_{r,R}(y,z)\, \sigma(z) \Big)\, \mathrm{d}y\, \mathrm{d}z \\
&\quad - \frac{1}{2} \hat{\omega}_{0000} \hat{n}_0. \\
&= \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} (\sigma(y) - \hat{n}_0 l^{-3})\, w_{r,R}(y,z)\, (\sigma(z) - \hat{n}_0 l^{-3})\, \mathrm{d}y\, \mathrm{d}z - \frac{1}{2} \hat{\omega}_{0000} \hat{n}_0. \\
&\geq \frac{1}{2} \Big\| nl^{-3} - \sigma \Big\|_{r,R}^2 + \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} (\sigma(y) - nl^{-3})\, w_{r,R}(y,z)\, \hat{n}_+ l^{-3}\, \mathrm{d}y\, \mathrm{d}z - \frac{1}{2} \hat{\omega}_{0000} \hat{n}_0. \\
&\geq \frac{1}{2}(1-\varepsilon') \Big\| nl^{-3} - \sigma \Big\|_{r,R}^2 - \frac{1}{2\varepsilon'} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \hat{n}_+ l^{-3}\, w_{r,R}(y,z)\, \hat{n}_+ l^{-3}\, \mathrm{d}y\, \mathrm{d}z - \frac{1}{2} \hat{\omega}_{0000} \hat{n}_0. \\
&= \frac{1}{2}(1-\varepsilon') \Big\| nl^{-3} - \sigma \Big\|_{r,R}^2 - \frac{1}{2\varepsilon'}\, \hat{\omega}_{0000}\, \hat{n}_+^2 - \frac{1}{2} \hat{\omega}_{0000} \hat{n}_0,
\end{aligned}$$

where the fact is used that $\omega_{r,R}$ defines a positive integral operator and therefore, one has the Cauchy-Schwarz inequality (4.36). Because of the bound $0 \leq \hat{\omega}_{0000} \leq 4\pi R^2 l^{-3}$ (see equation (4.16)), the desired result (4.41) holds. □

4.5 A-priori Estimates

In this section a-priori bounds are proven that are needed to estimate the subleading part of the Hamiltonian that is considered in section 4.4.

In doing so, Lemma 4.7 is used to bound the Hamiltonian from below by the Hamiltonian of the two component Bose gas of [37]. This way, one can transfer their a-priori bounds on the kinetic energy and on excitations to this case.

In addition, a-priori bounds on non-neutrality and Coulomb repulsion are needed. Since this bound is deduced by estimating $\langle \tilde{H}_{r,R} \rangle$ from below, it unfortunately cannot be subleading. However, it will be subleading when multiplied with a damping factor ε' or M^{-2} which will prove to be sufficient.

The first a-priori bound shows that asymptotically almost all of the particles will be in the condensate.

Lemma 4.19. *Let $C_1 > 0$ be the constant from* (4.9)*. Suppose $\langle \tilde{H} \rangle \leq 0$ and $C_1 N l^3 \leq \varepsilon^3$, then one has*

$$n \leq C \langle \hat{n}_0 \rangle ,$$

and

$$n^{5/4} \leq \langle \hat{n}_0 \rangle^{5/4} \Big(1 + C\varepsilon^{-1} (N^{2/5} l) N^{-1/24} \Big).$$

Proof. First, use Lemma 4.7 to transfer an a-priori bound on the number of excited particles from [37] to this case. Let $T_i = \gamma_{\varepsilon,t} \mathcal{K}_i - \gamma_{\varepsilon,t} \varepsilon \, \Delta_{i,\mathrm{Neu}}$ and $w = w_R$ as defined in (4.7). By equation (4.13), one can estimate

$$0 \geq \Big(\psi, \tilde{H} \psi \Big) = \Big(\psi, H^{(N)}_{w_R} \psi \Big) \geq \frac{1}{2} \Big(\psi \otimes \psi, \mathcal{H}^{(2N)}_{w_R} \psi \otimes \psi \Big).$$

Therefore, Corollary 6.4 of [37] yields $\langle \hat{n}_+ \rangle \leq C n \varepsilon^{-1} n^{1/3} l$. Since $n^{1/3} l \leq N^{1/3} l = (N^{2/5} l) N^{-1/15}$ this implies

$$\langle \hat{n}_0 \rangle = n - \langle \hat{n}_+ \rangle \geq n \Big(1 - C\varepsilon^{-1} n^{1/3} l \Big) \geq \Big(1 - C C_1^{-1/3} \Big) n = C^{-1} n,$$

by the choice of C_1 in (4.9) (see Lemma 11.2 of [37]). One arrives at the second equation of the lemma by expressing $n^{5/4} = n^{5/8} n^{5/8}$ in terms of $\hat{n}_0$ and $\hat{n}_+$ and using the subadditivity of the root. □

Lemma 4.20 (Estimates on the kinetic energy and excitations)**.** *Given that $\langle \tilde{H}_{r,R} \rangle \leq 0$ and assuming $C_1 \varepsilon \omega(t)^2 \leq nl$ and $C_1 N l^3 \leq \varepsilon^3$ for the constant $C_1 > 0$ from* (4.9)*, the following a-priori bounds hold.*

$$\left\langle \sum_{i=1}^{N} \mathcal{K}_i \right\rangle \leq C n^{5/4} l^{-3/4} \varepsilon^{-1/2} t^{-2} (nl)^{1/4}, \tag{4.42}$$

$$\langle \hat{n}_+ \rangle \leq C \varepsilon^{-3/2} t^{-2} (nl)^{3/2}. \tag{4.43}$$

Proof. These bounds are proven in [37], so Lemma 4.7 can be used to get the same result in this case. Set $T_i = \gamma_{\varepsilon,t}\mathcal{K}_i - \frac{1}{2}\gamma_{\varepsilon,t}\varepsilon\,\Delta_{i,\mathrm{Neu}}$ and $w = w_{r,R}$ to start from equation (4.13)

$$0 \geq \Big(\psi, \tilde{H}_{r,R}\psi\Big) = \Big(\psi, H^{(N)}_{w_{r,R}}\psi\Big) \geq \frac{1}{2}\Big(\psi\otimes\psi, \mathcal{H}^{(2N)}_{w_{r,R}}\psi\otimes\psi\Big).$$

According to Lemma 9.1 of [37] and since $(\psi,\psi) = 1$, one then has

$$\left(\psi\otimes\psi, \sum_{i=1}^{2N}\mathcal{K}_i\,\psi\otimes\psi\right) = 2\left(\psi, \sum_{i=1}^{N}\mathcal{K}_i\,\psi\right) \leq\, Cn^{5/4}l^{-3/4}\varepsilon^{-1/2}t^{-2}(nl)^{1/4}.$$

In the same way equation (4.43) is derived. □

Lemma 4.21 (Estimate on non-neutrality and Coulomb repulsion)**.** *Given that* $\langle\tilde{H}_{r,R}\rangle \leq 0$ *and assuming* $C_1\varepsilon\omega(t)^2 \leq nl \leq \varepsilon^{-4}(N^{2/5}l)^{10}$ *and* $C_1Nl^3 \leq \varepsilon^3$ *for the constant* $C_1 > 0$ *from* (4.9)*, the a-priori bound holds*

$$\begin{aligned}\Big\|nl^{-3} - \sigma\Big\|^2_{r,R} + \Big\langle\sum_{pq\mu\nu\neq 0}\hat{\omega}_{pq\mu\nu}\,a^*_pa^*_qa_\mu a_\nu\Big\rangle\\ \leq\, Cn^{5/4}l^{-3/4}\Big(\varepsilon^{-3/2}t^{-2}(nl)^{5/4} + K(\varepsilon,t,N,l)\Big).\end{aligned} \tag{4.44}$$

Here, $K(\varepsilon,t,N,l) = C\sum_{i=1}^m \varepsilon^{-a_i}t^{-b_i}(N^{2/5}l)^{c_i}N^{-d_i}$ *with* $d_i > 0$ *for all* i *and* $m\in\mathbb{N}$*.*

Proof. By equation (4.28) of Theorem 4.11 and the bound (4.20) for the main part of the Hamiltonian, one has

$$\begin{aligned}\Big\langle\tilde{H}_{r,R}\Big\rangle \geq\; & -Cn^{5/4}l^{-3/4} - C\varepsilon^{-1}t^{-22}nl^{-1}\\ & + \frac{1}{2}(1-3\varepsilon')\Big\|nl^{-3}-\sigma\Big\|^2_{r,R} + \frac{1}{2}(1-2\varepsilon')\Big\langle\sum_{pq\mu\nu\neq 0}\hat{\omega}_{pq\mu\nu}\,a^*_pa^*_qa_\mu a_\nu\Big\rangle\\ & - \Big(1+\frac{1}{2\varepsilon'}\Big)4\pi R^2l^{-3}\left\langle\hat{n}_+^2\right\rangle - \Big(5+\frac{2}{\varepsilon'}\Big)4\pi R^2l^{-3}n\left\langle\hat{n}_+ + 1\right\rangle\\ & - \sqrt{2}\Big\|nl^{-3}-\sigma\Big\|_{r,R}r^{-1/2}\left\langle\hat{n}_+\right\rangle \,-\, \varepsilon'r^{-1}\left\langle\hat{n}_+\right\rangle\end{aligned}$$

By estimating

$$\sqrt{2}\Big\|nl^{-3}-\sigma\Big\|_{r,R}r^{-1/2}\left\langle\hat{n}_+\right\rangle \leq \varepsilon'\Big\|nl^{-3}-\sigma\Big\|^2_{r,R} + \frac{1}{2\varepsilon'}r^{-1}\left\langle\hat{n}_+\right\rangle^2,$$

and choosing ε' as a sufficiently small constant, one then arrives at

$$\begin{aligned}\Big\langle\tilde{H}_{r,R}\Big\rangle \geq & - Cn^{5/4}l^{-3/4} - C\varepsilon^{-1}t^{-22}nl^{-1} - CR^2l^{-3}n\left\langle\hat{n}_+ + 1\right\rangle - Cr^{-1}\left\langle\hat{n}_+\right\rangle - Cr^{-1}\left\langle\hat{n}_+\right\rangle^2\\ & + \frac{1}{4}\Big\|nl^{-3}-\sigma\Big\|^2_{r,R} + \frac{1}{4}\Big\langle\sum_{pq\mu\nu\neq 0}\hat{\omega}_{pq\mu\nu}\,a^*_pa^*_qa_\mu a_\nu\Big\rangle.\end{aligned}$$

Note, that it is clear now, why the operator inequality of Lemma 4.16 is needed. Because of it, one has the term $Cr^{-1}\langle \hat{n}_+\rangle^2$ that can easily be controlled by using equation (4.43). $Cr^{-1}\langle \hat{n}_+^2\rangle$ could not have been controlled, however, as there is no good bound on $\langle \hat{n}_+^2\rangle$, yet.

Choosing $r = (nl)^{-1/2}l^{3/2}$ and $R \leq l$, because of the a-priori bound (4.43) the inequality holds

$$\begin{aligned}\left\langle \tilde{H}_{r,R}\right\rangle \geq & - Cn^{5/4}l^{-3/4}\Big(\varepsilon^{-3/2}t^{-2}(nl)^{5/4} + K(\varepsilon,t,N,l)\Big) \\ & + \frac{1}{4}\Big\|nl^{-3} - \sigma\Big\|^2_{r,R} + \frac{1}{4}\left\langle \sum_{pq\mu\nu\neq 0} \hat{\omega}_{pq\mu\nu}\, a_p^* a_q^* a_\mu a_\nu \right\rangle,\end{aligned}$$

where $K(\varepsilon,t,N,l) = C\sum_{i=1}^m \varepsilon^{-a_i}t^{-b_i}(N^{2/5}l)^{c_i}N^{-d_i}$ with $d_i > 0$ for all i and $m \in \mathbb{N}$. Here, the assumption is used that $C_1\varepsilon\omega(t)^2 \leq nl \leq \varepsilon^{-4}(N^{2/5}l)^{10}$ and $l = N^{-2/5+\delta_l}$ for some small $\delta_l > 0$. The lemma follows since $\langle \tilde{H}_{r,R}\rangle \leq 0$. □

4.6 Bound on the Excitations

In order to get an asymptotically sharp lower bound on the ground state energy, a better bound on the Coulomb repulsion term is needed than the one of equation (4.44). In this section this better bound is proven by showing that $\left\langle \hat{n}_+^2\right\rangle \sim \langle \hat{n}_+\rangle^2$. Lemmas 4.13 and 4.20 then yield the upper bound for the Coulomb repulsion.

As in [36] and [37], $\langle \hat{n}_+^2\rangle$ is not bounded for a general state ψ with negative energy. Instead, the existence of a state ψ' with a similar energy is proven such that $\hat{n}_+$ is sufficiently localized. To do this, the method of localizing large matrices developed in [36] is used. One thereby has to deal with the problem that the error of the energy can only be controlled by the Coulomb repulsion term that one actually wants to bound. However, for this purpose the bound (4.44) suffices even though it is greater than the leading order term. This is because one has an additional damping factor of M^{-2} in the error which renders it subleading, where $M \in \mathbb{N}$ is such that $\varepsilon^{-3/2}t^{-2}(nl)^{3/2} \in [M, M+1)$.

In the following lemma $\hat{n}_+$ is localized. Then, in a second lemma the error of this localization is estimated (similar to [36]).

Lemma 4.22. *Suppose $C_1\varepsilon\omega(t)^2 \leq nl$ and $C_1Nl^3 \leq \varepsilon^3$, where $C_1 > 0$ is the constant from* (4.9)*, and suppose ψ is a normalized wave function such that*

$$\left(\psi, \tilde{H}_{r,R}\psi\right) \leq -M^{-2}(|d_1(\psi)| + |d_2(\psi)|). \tag{4.45}$$

Then, there exists another normalized wave function ψ', that is a superposition of eigenfunctions of $\hat{n}_+$ with eigenvalue less than CM only, such that

$$\left(\psi, \tilde{H}_{r,R}\psi\right) \geq \left(\psi', \tilde{H}_{r,R}\psi'\right) - M^{-2}(|d_1(\psi)| + |d_2(\psi)|). \tag{4.46}$$

The localization error $M^{-2}(|d_1(\psi)| + |d_2(\psi)|)$ is defined and estimated in Lemma 4.23.

Proof. Recall that ψ is an eigenfunction of $\hat{n}$ with eigenvalue n. To apply the appropriate theorem of [36], expand $\psi = \sum_{m=0}^{n} c_m v_m$, where each v_m is a normalized eigenfunction of $\hat{n}_+$ with eigenvalue $m \in \{0, 1, \ldots, n\}$. Then, define

$$\mathcal{A}_{mm'} = \left(v_m, \tilde{H}_{r,R} v_{m'}\right)$$

for $m \in \{0, 1, \ldots, n\}$ and the corresponding matrix $\mathcal{A} := (\mathcal{A}_{mm'})_{0 \leq m, m' \leq n}$. Note that it is Hermitian. Applying Theorem A.1 of [36] to the matrix $\mathcal{A}$ and the vector $(c_0, \ldots, c_n)$ yields another wave function ψ' satisfying (4.46) that is a superposition of $v_{m+1}, \ldots, v_{m+M}$ for some $m \in \{0, \ldots, n\}$. The error term only includes d_1 and d_2 as no term in the Hamiltonian $\tilde{H}_{r,R}$ can change the number of excited particles by more than two. Here, it is assumed $M \geq 3$ which is true for a sufficiently small $t > 0$ since $nl \geq C_1 \varepsilon \omega(t)^2$.

Since one has $(\psi', \tilde{H}_{r,R} \psi') \leq 0$ due to equations (4.45) and (4.46) one can apply Lemma 4.20. Therefore, the estimate holds $(\psi', \hat{n}_+ \psi') \leq CM$ implying $m \leq CM$ and so, the proof is finished. □

Lemma 4.23. *Given that the assumptions of Lemma 4.22 are satisfied, one can bound the error in the case* $C_1 \varepsilon \omega(t)^2 \leq nl \leq \varepsilon^{-4} (N^{2/5} l)^{10}$ *by*

$$M^{-2}(|d_1(\psi)| + |d_2(\psi)|) \leq C \varepsilon^{-1} n l^{-1} + C \langle \hat{n}_0 \rangle^{5/4} l^{-3/4} K(\varepsilon, t, N, l), \tag{4.47}$$

where $K(\varepsilon, t, N, l) = C \sum_{i=1}^{\tilde{m}} \varepsilon^{-a_i} t^{-b_i} (N^{2/5} l)^{c_i} N^{-d_i}$ *with* $d_i > 0$ *for all* i *and* $\tilde{m} \in \mathbb{N}$.

The estimate of this lemma is proven separately for d_1 and d_2.

Proof of the estimate for d_1. The error term d_1 equals $(\psi, \tilde{H}_{r,R}(1)\psi)$ where $\tilde{H}_{r,R}(1)$ consists of all the terms in $\tilde{H}_{r,R}$ which contain exactly one or exactly three $a_0^{\#}$. These terms are bounded in Lemmas 4.14 and 4.17 from below. The same proof actually works for the upper bounds as well. Therefore, one has the bound

$$|d_1(\psi)| \leq C R^2 l^{-3} n \langle \hat{n}_+ + 1 \rangle + C \langle \hat{n}_+ \rangle r^{-1} + \left\| n l^{-3} - \sigma \right\|_{r,R}^2 + \left\langle \sum_{pq\mu\nu \neq 0} \hat{\omega}_{pq\mu\nu} \, a_p^* a_q^* a_\mu a_\nu \right\rangle .$$

Then, one can estimate with Lemma 4.21

$$|d_1(\psi)| \leq C R^2 l^{-3} n \langle \hat{n}_+ + 1 \rangle + C \langle \hat{n}_+ \rangle r^{-1} + C n^{5/4} l^{-3/4} \Big(\varepsilon^{-3/2} t^{-2} (nl)^{5/4} + K(\varepsilon, t, N, l) \Big).$$

Inserting the bound for $\langle \hat{n}_+ \rangle$ from (4.43) and the choices $r = (nl)^{-1/2} l^{3/2}$ and $R \leq l$, one gets the upper bound

$$\begin{aligned} &C n l^{-1} \varepsilon^{-3/2} t^{-2} (nl)^{3/2} + C n^{5/4} l^{-3/4} \varepsilon^{-3/2} t^{-2} (nl)^{3/4} l^{1/2} \\ &\quad + C n l^{-1} \varepsilon^{-3/2} t^{-2} (nl)^{3/2} + C n^{5/4} l^{-3/4} K(\varepsilon, t, N, l). \\ &= C n l^{-1} \varepsilon^{-3/2} t^{-2} (nl)^{3/2} + C n^{5/4} l^{-3/4} \Big(\varepsilon^{-3/2} t^{-2} (nl)^{3/4} l^{1/2} + K(\varepsilon, t, N, l) \Big). \end{aligned}$$

Since $M^{-2} \leq 1$, the error term can finally be bounded

$$M^{-2}|d_1(\psi)| \leq Cnl^{-1}t^2\varepsilon^{3/2}(nl)^{-3/2} + Cn^{5/4}l^{-3/4}\Big(\varepsilon^{3/2}t^2(nl)^{-9/4}l^{1/2} + K(\varepsilon,t,N,l)\Big).$$

Therefore, by inserting $C_1\varepsilon\omega(t)^2 \leq nl \leq \varepsilon^{-4}(N^{2/5}l)^{10}$ and $l = N^{-2/5+\delta_l}$, for a small $\delta_l > 0$, the upper bound holds

$$M^{-2}|d_1(\psi)| \leq Cnl^{-1} + Cn^{5/4}l^{-3/4}K(\varepsilon,t,N,l),$$

and because of Lemma 4.19, the proof is finished. □

Proof of the estimate for d_2. The error term d_2 equals $(\psi, \tilde{H}_{r,R}(2)\psi)$ where $\tilde{H}_{r,R}(2)$ consists of all the terms in $\tilde{H}_{r,R}$ which contain exactly two $a_0^{\#}$ that are either both a_0^* or both a_0.

Consider the unitary transform $\mathcal{U}$ which maps the basis vectors u_p to iu_p, for $p \neq 0$, leaving u_0 invariant. Then, $\mathcal{U}a_p^*\mathcal{U}^* = \mathrm{i}a_p^*$, while $\mathcal{U}a_p\mathcal{U}^* = -\mathrm{i}a_p$. Therefore, $\mathcal{U}$ maps H_{main} to an operator which only differs from H_{main} by a minus sign in the term that is called $\tilde{H}_{r,R}(2)$. Since the bound (4.20) for H_{main} remains invariant under $\mathcal{U}$, one can conclude

$$|d_2(\psi)| \leq \left\langle \sum_{i=1}^{N} \gamma_{\varepsilon,t}\mathcal{K}_i + \sum_{pq\neq 0} \hat{\omega}_{pq,00}a_p^*a_qa_0^*a_0 \right\rangle + \gamma_{\varepsilon,t}^{-1/4}I_0n^{5/4}l^{-3/4} + C\varepsilon^{-1}t^{-22}nl^{-1}.$$

Using equations (4.42) and 4.30, one has

$$|d_2(\psi)| \leq Cn^{5/4}l^{-3/4}\varepsilon^{-1/2}t^{-2}(nl)^{1/4} + 4\pi R^2l^{-3}n\langle\hat{n}_+\rangle + Cn^{5/4}l^{-3/4} + C\varepsilon^{-1}t^{-22}nl^{-1}.$$

Multiplying with M^{-2} and inserting (4.43) yields

$$M^{-2}|d_2(\psi)| \leq C\varepsilon^{-1}nl^{-1}.$$

By Lemma 4.19 the proof is finished. □

4.7 Proof of Theorem 4.4

In this section the lower bound on the energy in Q_l is proven. Recall that $\langle\tilde{H}\rangle = (\psi, \tilde{H}\psi)$, for an eigenfunction $\psi \in H^1(\mathbb{R}^3)$ of $\hat{n}$ with eigenvalue n.

First of all, boxes with few or many particles are estimated by a lower bound which does not contribute to the ground state energy at leading order. Note that sections 4.2-4.6 are not needed for this purpose (except for Lemma 4.7).

Lemma 4.24. *Let $C_1 > 0$ be the constant from* (4.9)*. Suppose $C_1Nl^3 \leq \varepsilon^3$ as well as $C_1l < \varepsilon t^4$. If either $nl \leq C_1\varepsilon\omega(t)^2$ or $nl \geq \varepsilon^{-4}(N^{2/5}l)^{10}$, then*

$$\begin{aligned}\langle\tilde{H}\rangle \geq &- Ct^{-6}nl^{-1} - Ct^{-22}l^{-2} - C\varepsilon^{-1}t^{-8}n - C\langle\hat{n}_0\rangle^{5/4}l^{-3/4}\varepsilon^{-1}(N^{2/5}l)N^{-1/15}\\ &- C\langle\hat{n}_0\rangle^{5/3}l^{-1/3}\Big(\varepsilon^{1/6}(N^{2/5}l)^{-5/3} + \varepsilon^{-2}(N^{2/5}l)^{4/3}N^{-3/15}\Big).\end{aligned}$$

Proof. Since this case does not contribute to the leading order term one can just use Lemma 4.7 to estimate it by the corresponding Hamiltonian $\mathcal{H}_w^{(2N)}$ of the two component Bose gas [37]. Therefore, choose C_1 at least as large as in Lemma 9.1 of [37]. With $w := w_R$ as defined in (4.7) and $T_i := \gamma_{\varepsilon,t}\mathcal{K}_i - \frac{1}{2}\gamma_{\varepsilon,t}\varepsilon\,\Delta_{i,\mathrm{Neu}}$, equation (4.13) reads

$$\left(\psi, \tilde{H}\psi\right) = \left(\psi, H_{w_R}^{(N)}\psi\right) \geq \frac{1}{2}\left(\psi\otimes\psi, \mathcal{H}_{w_R}^{(2N)}\psi\otimes\psi\right).$$

By Lemmas 11.4 and 11.5 from [37], the Hamiltonian is bounded from below by

$$\begin{aligned}\langle\tilde{H}\rangle \geq &-Cn^{5/4}l^{-3/4}\varepsilon^{-3/4}(N^{2/5}l)N^{-1/15}\\ &-Cn^{5/3}l^{-1/3}\left(\varepsilon^{1/6}(N^{2/5}l)^{-5/3}+\varepsilon^{-2}(N^{2/5}l)^{4/3}N^{-3/15}\right).\\ &-Ct^{-6}nl^{-1}-Ct^{-22}l^{-2}-C\varepsilon^{-1}t^{-8}n.\end{aligned}$$

In case $nl \geq \varepsilon^{-4}(N^{2/5}l)^{10}$, the estimate has been used

$$\begin{aligned}2^{1/4}\gamma_{\varepsilon,t}I_0\,n^{5/4}l^{-3/4} &\leq Cn^{5/3}l^{-1/3}(nl)^{-5/12} \leq Cn^{5/3}l^{-1/3}\varepsilon^{5/3}(N^{2/5}l)^{-50/12}\\ &\leq Cn^{5/3}l^{-1/3}\varepsilon^{1/6}(N^{2/5}l)^{-5/3}.\end{aligned}$$

Then, the lemma follows because of Lemma 4.19. □

To bound $\langle\tilde{H}\rangle$ from below all of the results of sections 4.2-4.6 are combined.

Proof of Theorem 4.4. Since the other case has already been covered in Lemma 4.24, consider the case $C_1\varepsilon\omega(t)^2 \leq nl \leq \varepsilon^{-4}(N^{2/5}l)^{10}$. Furthermore, if $\langle\tilde{H}\rangle \geq 0$, the proof is finished. Thus, assume $\langle\tilde{H}\rangle \leq 0$. Then, one can make use of Lemma 4.19.

First of all, it has to be considered what happens if the conditions of Lemma 4.20 or Lemma 4.22 fail. So, suppose $\langle\tilde{H}_{r,R}\rangle \geq 0$. Using the fact that $r = (nl)^{-1/2}l^{3/2}$, one has by Lemma 4.6

$$\begin{aligned}\langle\tilde{H}\rangle &\geq -Cn^2(\varepsilon^{-3/2}r^{1/2}+r^2l^{-3})\\ &\geq -C\varepsilon^{-3/2}n^{5/4}l^{-3/4}(nl)^{1/2}l^{3/4}-Cnl^{-1}.\end{aligned}$$

As $nl \leq \varepsilon^{-4}(N^{2/5}l)^{10}$, one can get a bound of the desired form by Lemma 4.19. In the following, it is therefore assumed $\langle\tilde{H}_{r,R}\rangle \leq 0$. Note that this showed that the error of the short distance cutoff is subleading which is why it suffices to bound $\langle\tilde{H}_{r,R}\rangle$ from below instead of $\langle\tilde{H}\rangle$.

In case condition (4.45) for the localization of the number of excited particles is not satisfied, the expectation value $\langle\tilde{H}_{r,R}\rangle$ is bounded from below by the bound in (4.47). Therefore, it may be assumed that condition (4.45) is satisfied and thus, Lemma 4.22 can be applied. Then, there exists another normalized wave function ψ' with

$$\begin{aligned}\left(\psi, \tilde{H}_{r,R}\psi\right) &\geq \left(\psi', \tilde{H}_{r,R}\psi'\right) - M^{-2}(|d_1(\psi)|+|d_2(\psi)|)\\ &\geq \left(\psi', \tilde{H}_{r,R}\psi'\right) - C\varepsilon^{-1}nl^{-1} - C\langle\hat{n}_0\rangle^{5/4}l^{-3/4}K(\varepsilon,t,N,l), \qquad (4.48)\end{aligned}$$

such that

$$\langle \hat{n}_+ \rangle' \le C\varepsilon^{-3/2} t^{-2} (nl)^{3/2}, \tag{4.49}$$

$$\left\langle \hat{n}_+^2 \right\rangle' \le C\varepsilon^{-3} t^{-4} (nl)^3, \tag{4.50}$$

where the expectation value with respect to ψ' is denoted by $\langle \cdot \rangle'$ to distinguish it from the expectation value $\langle \cdot \rangle$ with respect to ψ.

By Theorem 4.8 and equation (4.29) of Theorem 4.11, one has

$$\begin{aligned} \tilde{H}_{r,R} \ \ge\ & -\gamma_{\varepsilon,t}^{-1/4} I_0 n^{5/4} l^{-3/4} - \frac{1}{2} \left\| nl^{-3} - \sigma \right\|_{r,R}^2 - 4\pi n l^{-1} \\ & + \frac{1}{2}(1-3\varepsilon') \left\| nl^{-3} - \sigma \right\|_{r,R}^2 + \left(\frac{1}{2} - \frac{1}{\varepsilon'} \right) \sum_{pq\mu\nu \ne 0} \hat{\omega}_{pq\mu\nu}\, a_p^* a_q^* a_\mu a_\nu \\ & - \left(1 + \frac{3}{2\varepsilon'} \right) 4\pi R^2 l^{-3} \hat{n}_+^2 \ - \varepsilon' 12\pi R^2 l^{-3} n \hat{n}_+ - 2\pi R^2 l^{-3} n \\ & - \frac{1}{\varepsilon'} 4\pi R^2 l^{-3} (2\hat{n}_+ + 1) - \frac{1}{\varepsilon'} r^{-1} \hat{n}_+ (\hat{n}_+ + 1). \end{aligned}$$

By Lemma 4.13, the lower bound holds

$$\begin{aligned} \tilde{H}_{r,R} \ge & -\gamma_{\varepsilon,t}^{-1/4} I_0 n^{5/4} l^{-3/4} - Cnl^{-1} - C\varepsilon' \left\| nl^{-3} - \sigma \right\|_{r,R}^2 \\ & - CR^2 l^{-3} \left(n + \varepsilon' n \hat{n}_+ + \frac{1}{\varepsilon'}(1+\hat{n}_+) + \left(1 + \frac{1}{\varepsilon'}\right) \hat{n}_+^2 \right) - Cr^{-1} \left(\frac{1}{\varepsilon'} \hat{n}_+ + \frac{1}{\varepsilon'} \hat{n}_+^2 \right). \end{aligned}$$

Since $r = (nl)^{-1/2} l^{3/2}$ and $R \le \omega(t)^{-1} l$ and because of the neutrality bound (4.44) and the bounds for excitations (4.49) and (4.50) it follows

$$\begin{aligned} \left\langle \tilde{H}_{r,R} \right\rangle' \ge & -\gamma_{\varepsilon,t}^{-1/4} I_0 n^{5/4} l^{-3/4} - Cnl^{-1} - \varepsilon' C n^{5/4} l^{-3/4} \left(\varepsilon^{-3/2} t^{-2} (nl)^{5/4} + K(\varepsilon, t, N, l) \right) \\ & - C\omega(t)^{-2} l^{-1} \left(\varepsilon' n\, \varepsilon^{-3/2} t^{-2} (nl)^{3/2} + \frac{1}{\varepsilon'} \left(1 + \varepsilon^{-3/2} t^{-2} (nl)^{3/2} \right) + \left(1 + \frac{1}{\varepsilon'} \right) \varepsilon^{-3} t^{-4} (nl)^3 \right) \\ & - C l^{-3/2} (nl)^{1/2} \left(\frac{1}{\varepsilon'}\, \varepsilon^{-3/2} t^{-2} (nl)^{3/2} + \frac{1}{\varepsilon'}\, \varepsilon^{-3} t^{-4} (nl)^3 \right). \end{aligned}$$

Finally, choose $\varepsilon' := l^{1/4}$ to get

$$\begin{aligned} \left\langle \tilde{H}_{r,R} \right\rangle' \ge & -\gamma_{\varepsilon,t}^{-1/4} I_0 n^{5/4} l^{-3/4} - Cnl^{-1} - C n^{5/4} l^{-3/4} \left(\varepsilon^{-3/2} t^{-2} (nl)^{5/4} l^{1/4} + K(\varepsilon, t, N, l) \right) \\ & - C n^{5/4} l^{-3/4} \left(\varepsilon^{-3/2} (nl)^{5/4} l^{1/4} + \varepsilon^{-5/4} l^{3/4} + \varepsilon^{-3/2} (nl)^{1/4} l^{3/4} + \varepsilon^{-3} t^{-4} (nl)^{7/4} l^{3/4} \right) \\ & - C n^{5/4} l^{-3/4} \left(\varepsilon^{-3/2} t^{-2} (nl)^{3/4} l^{1/4} + \varepsilon^{-3} t^{-4} (nl)^{9/4} l^{1/4} \right). \end{aligned}$$

Therefore, by equation (4.48), Lemma 4.19 and by inserting $nl \le \varepsilon^{-4} (N^{2/5} l)^{10}$ and $l = N^{-2/5+\delta_l}$ for a small $\delta_l > 0$, the desired lower bound on the energy in a small cube is concluded. □

Appendix A

Localization of the Hamiltonian

A.1 Putting the System into One Cube Q_L

Since the polaron system is unstable (i.e. the ground state energy cannot be bounded from below by $-CN$), it implodes for $N \to \infty$. This is why one can put the whole system in a box $Q_L = (-L/2, L/2)^3$, where $L \to 0$, and still get the correct leading order coefficient. Since later on it is necessary that the volume is finite, the Hamiltonian $H^{(N)}$ is localized in this section into one "large" cube Q_L.

The procedure of localizing the potential is very similar to that in [36] since for this purpose it is not actually needed that the background charge density is the indicator function $\rho 1_{Q_L}$. Everything works just as well with a general real background function $\sigma \in L^1(\mathbb{R}^3)$ fulfilling $D(\sigma, \sigma) < \infty$.

As in [36] the sliding method developed in [11] is used to decouple the Coulomb interaction of different boxes. In this case, however, the localization has to be done twice since one has two different relevant length scales. Since the two component Bose gas has the same length scales, one can largely proceed as in [37]. For this purpose, now the necessary notions are introduced.

First, choose the localization functions $\theta, \Theta \in C_c^4(\mathbb{R}^3)$ as it is done in Section 4 of [37]. They are approximations to step functions with parameter $t \in (0, \frac{1}{2})$. Later t will tend to zero slowly as $N \to \infty$. (E.g. $t \propto (\log N)^{-1}$ would work though it is not a very good choice.) The properties of θ and Θ chosen in [37] are

(i) $0 \leq \theta(z), \Theta(z) \leq 1$, $\theta(z) = \theta(-z)$ and $\Theta(z) = \Theta(-z)$ for all $z \in \mathbb{R}^3$.

(ii) $\operatorname{supp} \theta \subset Q_{1-t}$ whereas $\operatorname{supp} \Theta \subset Q_{1+t}$.

(iii) $\theta(z) = 1$ if $z \in Q_{1-2t}$ and $\Theta(z) = 1$ if $z \in Q_{1-t}$.

(iv) For $i \in \{1, 2, 3\}$, the derivatives of order i of $\theta, \sqrt{1-\theta^2}$ and Θ are bounded by Ct^{-i} uniformly.

(v) One has $\sum_{k \in \mathbb{Z}^3} \Theta(z-k)^2 = 1$ for any $z \in \mathbb{R}^3$. (A.1)

Also define the normalization constants $\gamma := (\int_{\mathbb{R}^3} \theta(z)^2 \, \mathrm{d}z)^{-1}$ and $\tilde{\gamma} := (\int_{\mathbb{R}^3} \Theta(z)^4 \, \mathrm{d}z)^{-1}$. One has

$$1 \leq \gamma \leq (1-2t)^{-3} \qquad \text{and} \qquad (1+t)^{-3} \leq \tilde{\gamma} \leq (1-t)^{-3}. \tag{A.2}$$

The Coulomb interaction is very far reaching. However, the method developed in [11] decouples the interaction of the different cubes and thus, reduces the problem to estimate the energy of a single small cube $Q_l(kl)$ from below.

Define the Yukawa potential

$$Y_m(z) = \frac{\mathrm{e}^{-m|z|}}{|z|}, \tag{A.3}$$

for $m \geq 0$. Furthermore, let $\chi = \theta$ or $\chi = \Theta^2$ and let $\gamma_\chi = \gamma$ or $\gamma_\chi = \tilde{\gamma}$, respectively.

Lemma A.1 (Localization of the potential)**.** *One has for all $t < 1/2$, for all $x_1, x_2, ..., x_N \in \mathbb{R}^3$, all $m \geq 0$, all $\lambda > 0$ and all $\sigma \in L^1(\mathbb{R}^3)$, fulfilling $D(\sigma, \sigma) < \infty$,*

$$\begin{aligned} &\sum_{1 \leq i < j \leq N} Y_m(x_i - x_j) - \sum_{i=1}^N \int_{\mathbb{R}^3} \sigma(y) Y_m(y - x_i) \, \mathrm{d}y + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \sigma(y) Y_m(y-z) \sigma(z) \, \mathrm{d}y \, \mathrm{d}z \\ &\geq \gamma_\chi \int_{\mathbb{R}^3} \Bigg(\sum_{1 \leq i < j \leq N} \chi\Big(\frac{x_i}{\lambda} - \mu\Big) Y_{m + \frac{\omega(t)}{\lambda}}(x_i - x_j) \chi\Big(\frac{x_j}{\lambda} - \mu\Big) \\ &\qquad - \sum_{i=1}^N \int_{\mathbb{R}^3} \sigma(y) \chi\Big(\frac{y}{\lambda} - \mu\Big) Y_{m+\frac{\omega(t)}{\lambda}}(y - x_i) \chi\Big(\frac{x_i}{\lambda} - \mu\Big) \, \mathrm{d}y \\ &\qquad + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \sigma(y) \chi\Big(\frac{y}{\lambda} - \mu\Big) Y_{m+\frac{\omega(t)}{\lambda}}(y-z) \chi\Big(\frac{z}{\lambda} - \mu\Big) \sigma(z) \, \mathrm{d}y \, \mathrm{d}z \Bigg) \, \mathrm{d}\mu - \frac{N\omega(t)}{2\lambda}, \end{aligned}$$

where $\omega(t) = C_\omega t^{-4}$ and $\omega(t) \geq 1$ if $t < 1/2$.

Proof. Similar to the proof of Lemma 3.1 in [36], note that

$$\int_{\mathbb{R}^3} \gamma_\chi \, \chi(y+\mu) Y_{\lambda m + \omega}(y-z) \chi(z+\mu) \, \mathrm{d}\mu = h(y-z) Y_{\lambda m + \omega}(y-z),$$

with the convolution $h = \gamma_\chi \chi * \chi$. One has $h(0) = \gamma_\chi \int_{\mathbb{R}^3} \chi(\mu)^2 \, \mathrm{d}\mu = 1$ by the choice of γ_χ. Therefore, h fulfills the assumptions of Lemma 2.1 in [11]. This lemma states that the Fourier transform of $F(z) = Y_{\lambda m}(z) - h(z) Y_{\lambda m + \omega}(z)$ is positive if ω is large enough. As it is done in [36], one can indeed choose $\omega(t) = C_\omega t^{-4}$. In particular, it is independent of m and λ. Therefore, the bound is deduced

$$\begin{aligned} &\sum_{i<j} F(x_i - x_j) - \lambda^3 \sum_{i=1}^N \int_{\mathbb{R}^3} \sigma(\lambda y) F(y - x_i) \, \mathrm{d}y + \frac{\lambda^6}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \sigma(\lambda y) F(y-z) \sigma(\lambda z) \, \mathrm{d}y \, \mathrm{d}z \\ &= \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \Big(\sum_{i=1}^N \delta(y - x_i) - \lambda^3 \sigma(\lambda y) \Big) F(y-z) \Big(\sum_{i=1}^N \delta(z - x_i) - \lambda^3 \sigma(\lambda z) \Big) \, \mathrm{d}y \, \mathrm{d}z \\ &\quad - \frac{1}{2} \sum_{i=1}^N F(0) \ \geq \ -\frac{N\omega}{2}. \end{aligned}$$

Since this estimate holds for all σ, all $\lambda > 0$ and all $m \geq 0$, the lemma is concluded after rescaling. □

Let Δ_{D} denote the Dirichlet Laplacian in the cube $Q_L = (-L/2, L/2)^3$. For $\sigma \in L^1(\mathbb{R}^3)$, with $D(\sigma,\sigma) < \infty$, define the Hamiltonian

$$H_{N,L}^{(\sigma)} := \sum_{i=1}^{N} -\Delta_{i,\mathrm{D}} + \tilde{\gamma} \sum_{1\leq i<j\leq N} Y_{\frac{2\omega(t)}{L}}(x_i - x_j) - \tilde{\gamma}\sum_{i=1}^{N}\int_{Q_L} \sigma(y) Y_{\frac{2\omega(t)}{L}}(y - x_i)\,\mathrm{d}y + \tilde{\gamma}\frac{1}{2}\int_{Q_L}\int_{Q_L} \sigma(y) Y_{\frac{2\omega(t)}{L}}(y-z)\sigma(z)\,\mathrm{d}y\,\mathrm{d}z$$

acting on the space $L^2(Q_L^N)$. Define

$$E_L(N) := \inf_{\sigma} \inf \operatorname{spec} H_{N,L}^{(\sigma)}.$$

Theorem A.2 (Reducing the problem to one cube Q_L)**.** *One has the bound*

$$E_1^{(b)}(N) \geq E_L(N) - N^{7/5}\Big(Ct^{-2}(N^{1/5}L)^{-2} + Ct^{-4}(N^{1/5}L)^{-1}N^{-1/5}\Big).$$

Proof. For $\mu \in \mathbb{R}^3$ define $\Theta_\mu(x) = \Theta(2x/L - \mu)$. The length scale $L/2$ is used since $\operatorname{supp}\Theta_\mu \subset \mu + [(-1-t)L/4, (1+t)L/4] \subset Q_L(\mu)$ which is just what one wants to end up with. Then, by (A.1)

$$\sum_{q\in\mathbb{Z}^3} \Theta_{\mu+q}^2(x) = 1.$$

By Lemma A.1 with $\lambda = L/2$ and $m = 0$ one has

$$\begin{aligned} &\sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|} - \sum_{i=1}^{N}\int_{\mathbb{R}^3} \frac{\sigma(y)}{|y - x_i|}\,\mathrm{d}y + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\sigma(y)\sigma(z)}{|y-z|}\,\mathrm{d}y\,\mathrm{d}z \\ &\geq \tilde{\gamma}\sum_{k\in\mathbb{Z}^3}\int_{Q_1}\Bigg(\sum_{1\leq i<j\leq N} \Theta_{k+\mu}^2(x_i) Y_{\frac{2\omega(t)}{L}}(x_i - x_j)\Theta_{k+\mu}^2(x_j) \\ &\qquad - \sum_{i=1}^{N}\int_{\mathbb{R}^3} \sigma(y)\Theta_{k+\mu}^2(y) Y_{\frac{2\omega(t)}{L}}(y - x_i)\Theta_{k+\mu}^2(x_i)\,\mathrm{d}y \\ &\qquad + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \sigma(y)\Theta_{k+\mu}^2(y) Y_{\frac{2\omega(t)}{L}}(y-z)\Theta_{k+\mu}^2(z)\sigma(z)\,\mathrm{d}y\,\mathrm{d}z\Bigg)\,\mathrm{d}\mu - \frac{N\omega(t)}{L}. \end{aligned} \tag{A.4}$$

Now, a redundant sum is introduced over the square of

$$F_{\mathbf{q},\mu}(x) = \Theta_{q_1+\mu}(x_1)\cdots\Theta_{q_N+\mu}(x_N), \qquad \text{for } \mathbf{q} = (q_1,\ldots,q_N) \in (\mathbb{Z}^3)^N \text{ and } x \in (\mathbb{R}^3)^N.$$

Then, the right side of (A.4) becomes

$$\tilde{\gamma} \sum_{k\in\mathbb{Z}^3} \sum_{\mathbf{q}\in\mathbb{Z}^{3N}} \int_{Q_1} F_{\mathbf{q},\mu}(x) \Bigg(\sum_{1\le i<j\le N} \delta_{q_i,k} Y_{\frac{2\omega(t)}{L}}(x_i - x_j)\delta_{q_j,k} \\ - \sum_{i=1}^N \int_{\mathbb{R}^3} \sigma(y)\Theta_{k+\mu}^2(y) Y_{\frac{2\omega(t)}{L}}(y - x_i)\delta_{q_i,k}\,\mathrm{d}y \\ + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \sigma(y)\Theta_{k+\mu}^2(y) Y_{\frac{2\omega(t)}{L}}(y - z)\Theta_{k+\mu}^2(z)\sigma(z)\,\mathrm{d}y\,\mathrm{d}z \Bigg) F_{\mathbf{q},\mu}(x)\,\mathrm{d}\mu - \frac{N\omega(t)}{L}.$$

As in the proof of Theorem 4.2 in [37], the estimate $-\Delta \ge \sum_{k\in\mathbb{Z}^3} \Theta_{k+\mu}(-\Delta)\Theta_{k+\mu} - C(tL^{-2})$ is used to get

$$\sum_{i=1}^N -\Delta_i \ge \sum_{\mathbf{q}\in(\mathbb{Z}^3)^N} \int_{Q_1} F_{\mathbf{q},\mu}(x) \sum_{i=1}^N (-\Delta_i) F_{\mathbf{q},\mu}(x)\,\mathrm{d}\mu - CN(tL)^{-2}.$$

Then, by interchanging the sums and the infima we have

$$E_1^{(b)}(N) \ge \sum_{\mathbf{q}\in(\mathbb{Z}^3)^N} \int_{Q_1} F_{\mathbf{q},\mu}(x)^2 \sum_{k\in\mathbb{Z}^3} \inf_\sigma \inf \operatorname{spec} \tilde{H}_{\mathbf{q},k,\mu}\,\mathrm{d}\mu - N\omega(t)L^{-1} - CN(tL)^{-2}, \quad \text{(A.5)}$$

where the Hamiltonian is defined by

$$\tilde{H}_{\mathbf{q},k,\mu} = \sum_{i=1}^N \delta_{q_i,k}\,\Delta_{i,\mathrm{D}}^{(k+\mu)} + \tilde{\gamma} \sum_{1\le i<j\le N} \delta_{q_i,k} Y_{\frac{2\omega(t)}{L}}(x_i - x_j)\delta_{q_j,k} \\ - \sum_{i=1}^N \int_{Q_L(k+\mu)} \sigma(y) Y_{\frac{2\omega(t)}{L}}(y - x_i)\delta_{q_i,k}\,\mathrm{d}y + \frac{1}{2}\iint_{(Q_L(k+\mu))^2} \sigma(y) Y_{\frac{2\omega(t)}{L}}(y - z)\sigma(z)\,\mathrm{d}y\,\mathrm{d}z\,,$$

acting only on functions for which space variables are in the cube Q_L about $k+\mu$. Note that $0 \le \Theta \le 1_{Q_L}$ means that the $\Theta_{k+\mu}^2$ in the integral can be absorbed into the infimum over σ. The Hamiltonian $\tilde{H}_{\mathbf{q},k,\mu}$ is unitary equivalent to $H_{N,L}^{(\sigma)}$ with N replaced by $N_k(\mathbf{q}) = |\{i:\ q_i = k\}|$. Therefore, equation (A.5) becomes

$$E_1^{(b)}(N) \ge \sum_{\mathbf{q}\in(\mathbb{Z}^3)^N} \int_{Q_1} F_{\mathbf{q},\mu}(x)^2 \sum_{k\in\mathbb{Z}^3} E_L(N_k(\mathbf{q}))\,\mathrm{d}\mu - N\omega(t)L^{-1} - CN(tL)^{-2},$$

where one has $\sum_{k\in\mathbb{Z}} N_k(\mathbf{q}) = N$ for any $\mathbf{q} \in (\mathbb{Z}^3)^N$. It remains to show that $E_L(N)$ is sub-additive in N. Then, the theorem follows.

For this purpose, it is helpful to undo the linearization that has been introduced in Section 4.1. That is, for $\psi \in L^2(Q_L^N)$, consider the energy functional

$$\mathcal{E}_w^{(N)}[\psi] := \int_{Q_L^N} \left(\sum_{i=1}^N |\nabla_i\psi|^2 + \sum_{1\le i<j\le N} w(x_i,x_j)\,|\psi|^2 \right) \mathrm{d}x - D_w(\rho_\psi,\rho_\psi), \quad \text{(A.6)}$$

where $w(x, y) = Y_{2\omega(t)/L}(x - y)$ and

$$D_w(f, g) := \frac{1}{2} \iint_{Q_L \times Q_L} \overline{f(y)}\, w(y, z)\, g(z)\, \mathrm{d}y\, \mathrm{d}z\,.$$

By the same argument as in Section 4.1, one has

$$\inf_{\|\psi\|=1} \mathcal{E}_w^{(N)}[\psi] = \inf_{\sigma} \inf \operatorname{spec} H_{N,L}^{(\sigma)} = E_L(N).$$

For an N_1-particle wave function ψ_1 and an N_2-particle wave function ψ_2, a straightforward calculation shows

$$E_L(N_1 + N_2) \leq \mathcal{E}_w^{(N_1+N_2)}[\psi_1 \otimes \psi_2] = \mathcal{E}_w^{(N_1)}[\psi_1] + \mathcal{E}_w^{(N_2)}[\psi_2].$$

Taking the infimum over all ψ_1 and all ψ_2 proves the sub-additivity of $E_L(N)$. □

A.2 Reducing the problem to the length scale l of local condensation

As explained before the idea of the proof is to localize the problem to the small length scale $l \propto N^{-2/5+\delta_l}$ where most particles are in the condensate. This is where Bogolubov theory is applied. In this section a lower bound on the energy is derived in terms of a local Hamiltonian on Q_l.

One main difficulty that arises, is the question on how to split the kinetic energy $\sum_{i=1}^{N} -\Delta_{i,\mathrm{D}}$ into a low and a high momentum part. First of all, the kinetic energy between different small boxes is needed, as it gives rise to the term $\int_{\mathbb{R}^3} |\boldsymbol{\nabla}\Phi|^2\, \mathrm{d}x$ in (1.26). But then, the kinetic energy within each of the small boxes gives a positive contribution to the second term $-I_0 \int_{\mathbb{R}^3} |\Phi|^{5/2}\, \mathrm{d}x$ in (1.26). This difficulty was resolved by Lieb and Solovej in [37]. To quote their result on the localization of the kinetic energy the necessary notions are introduced.

For $\mu \in \mathbb{R}$, let $\mathcal{P}^{(\mu)}$ be the projection onto the subspace of $L^2(Q_l(\mu l))$ orthogonal to constants. The operator that is used to describe the kinetic energy in the small cube about μl is then given by

$$\mathcal{K}^{(\mu)} = \mathcal{P}^{(\mu)} \chi_l^{(\mu)} \frac{(-\Delta)^2}{-\Delta + (lt^6)^{-2}} \chi_l^{(\mu)} \mathcal{P}^{(\mu)},$$

where $\mathcal{P}^{(\mu)}$ is regarded as an operator acting on $L^2(\mathbb{R}^3)$. The localization function is

$$\chi_l^{(\mu)}(z) = \theta(z/l - \mu),$$

where θ was chosen in the beginning of Section A.1. As in [37], the kinetic energy between small boxes is measured by the quadratic form T induced by a lattice Laplacian which maps a function $S : \mathbb{Z}^3 \to \mathbb{R}$ to

$$T(S) = \sum_{\substack{k_1,k_2\in\mathbb{Z}^3\\ |k_1-k_2|=\sqrt{2}}} \frac{1}{12}(S(k_1) - S(k_2))^2 + \sum_{\substack{k_1,k_2\in\mathbb{Z}^3\\ |k_1-k_2|=\sqrt{3}}} \frac{1}{24}(S(k_1) - S(k_2))^2. \tag{A.7}$$

Define the particle number operator in the μ-th small cube

$$\hat{n}^{(\mu)}(x) = \sum_{i=1}^{N} 1_{Q_l(\mu l)}(x_i),$$

where $x \in (\mathbb{R}^3)^N$ and where 1_{Q_l} is the characteristic function of the cube Q_l. The number of particles in the condensate which are in the cube about μl is

$$\hat{n}_0^{(\mu)} = l^{-3} a^*(1_{Q_l(\mu l)})\, a(1_{Q_l(\mu l)}),$$

where the operators $a(u)$ and $a^*(u)$ in the Fock space $\bigoplus_{N=0}^{\infty} \bigotimes_{\mathrm{s}}^{N} L^2(\mathbb{R}^3)$ have been defined in the introduction for $u \in L^2(\mathbb{R}^3)$. Finally, the number of excited particles in the μ-th cube is given by

$$\hat{n}_+^{(\mu)} = \hat{n}^{(\mu)} - \hat{n}_0^{(\mu)}.$$

2

To turn to the localization of the kinetic energy, for a given wave function ψ, define the map $S_\mu^\psi : \mathbb{Z}^3 \to \mathbb{R}$,

$$S_\mu^\psi(k) = l^{-1}\Big(\Big(\langle \hat{n}_0^{(k+\mu)}\rangle + 1\Big)^{1/2} - 1\Big), \qquad \text{where} \qquad \langle \hat{n}_0^{(k+\mu)}\rangle = \Big(\psi, \hat{n}_0^{(k+\mu)}\psi\Big). \tag{A.8}$$

Now, quote Lemma 5.1 from [37]. Note that this result is not needed on the space $\bigotimes_{\mathrm{s}}^{N} L^2(\mathbb{R}^3 \times \{1,-1\})$ but only on $\bigotimes_{\mathrm{s}}^{N} L^2(\mathbb{R}^3 \times \{1\}) \cong \bigotimes_{\mathrm{s}}^{N} L^2(\mathbb{R}^3)$.

Lemma A.3 (Splitting the kinetic energy into low and high momentum part)**.** *Let* $\psi \in \bigotimes_{\mathrm{s}}^{N} L^2(\mathbb{R}^3)$ *with* $\int_{(\mathbb{R}^3)^N} |\psi|^2 \,\mathrm{d}x = 1$ *and* $\operatorname{supp}\psi \subset Q_L^N = (-L/2, L/2)^{3N}$, *then for all* $\varepsilon > 0$ *and* $t \in (0, \frac{1}{2})$,

$$\begin{aligned}&(1 + \varepsilon + Ct^3)\Big(\psi, \sum_{i=1}^{N} -\Delta_{i,\mathrm{D}}\psi\Big)\\ &\geq \int_{Q_1^3}\Bigg(\Big(\psi, \sum_{k\in\mathbb{Z}^3}\sum_{i=1}^{N}\Big(\mathcal{K}_i^{(k+\mu)} - \varepsilon\,\Delta_{i,\mathrm{Neu}}^{(k+\mu)}\Big)\psi\Big) + T(S_\mu^\psi)\Bigg)\,\mathrm{d}\mu - CL^3 l^{-5}.\end{aligned}$$

Here, $-\Delta_{\mathrm{Neu}}^{(\mu)}$ *is the Laplacian on the small cube* $Q_l(\mu l)$ *fulfilling the Neumann boundary condition.*

With this lemma, one can localize the Hamiltonian into many small cubes of size $l \ll L$. Later, it will be chosen $l \propto N^{-2/5+\delta_l}$ for a small $\delta_l > 0$. Define the Hamiltonian acting on functions in the small cube about μl

$$\begin{aligned}\tilde{H}^{(\mu)} = &\gamma_{\varepsilon,t} \sum_{i=1}^{N} \left(\mathcal{K}_i^{(\mu)} - \varepsilon\, \Delta_{i,\mathrm{Neu}}^{(\mu)} \right) + \sum_{1 \le i < j \le N} w_R^{(\mu)}(x_i, x_j) \\ &- \sum_{i=1}^{N} \int_{\mathbb{R}^3} \sigma(y) w_R^{(\mu)}(y, x_i)\, \mathrm{d}y + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \sigma(y) w_R^{(\mu)}(y, z) \sigma(z)\, \mathrm{d}y\, \mathrm{d}z\,,\end{aligned}$$

where $\gamma_{\varepsilon,t} = (1 + \varepsilon + Ct^3)^{-1}(\gamma\tilde{\gamma})^{-1}$ and where the interaction is given by

$$w_R^{(\mu)}(y, z) = \chi_l^{(\mu)}(y) Y_{R^{-1}}(y - z) \chi_l^{(\mu)}(z) = \chi_l^{(\mu)}(y) \frac{\mathrm{e}^{-|y-z|/R}}{|y - z|} \chi_l^{(\mu)}(z). \tag{A.9}$$

The localization function is $\chi_l^{(\mu)}(z) = \theta(z/l - \mu)$, with θ as of the beginning of Section A.1. The long distance cutoff is given by

$$R = \eta\, \omega(t)^{-1} l, \tag{A.10}$$

where $\omega(t) = C_\omega t^{-4}$ and $\eta = (1 + 2l/L)^{-1} \approx 1$ since $l \ll L$. Note that a small and unimportant mistake in [37] is corrected by introducing η.

Theorem A.4 (A lower bound in terms of the local Hamiltonian)**.** *The ground state energy $E_L(N)$ of the polaron system in the large cube is bounded below by*

$$E_L(N) \ge \gamma\tilde{\gamma} \inf_{\|\psi\|=1} \left\{ \inf_{\sigma} \left(\psi, \sum_{k \in \mathbb{Z}^3} \tilde{H}^{(k)} \psi \right) + \gamma_{\varepsilon,t}\, T(S_0^{\psi}) \right\} - L^3 l^{-5} - \frac{N\omega(t)}{2l}.$$

The infimum is taken over wave functions ψ is in the space

$$\mathcal{H}_0 := \left\{ \phi \in \textstyle\bigotimes_{\mathrm{s}}^{N} L^2(\mathbb{R}^3) \;\middle|\; \hat{n}^{(k)} \phi = 0 \text{ for } kl \notin \mathbb{Z}^3 \cap Q_{L+l} \right\}.$$

Proof. Apply Lemma A.1 with $\chi = \theta$, $m = 2\omega(t)/L$ and $\lambda = l$. Furthermore, use Lemma A.3. One then gets

$$\left(\psi, H_{N,L}^{(\sigma)} \psi\right) \ge \gamma\tilde{\gamma} \int_{Q_1} \left(\left(\psi, \sum_{k \in \mathbb{Z}^3} \tilde{H}^{(k+\mu)} \psi \right) + \gamma_{\varepsilon,t}\, T(S_\mu^{\psi}) \right) \mathrm{d}\mu - L^3 l^{-5} - \frac{N\omega(t)}{2l}.$$

One arrives at the theorem by commuting the infima and the integration and noting that they are independent of $\mu \in Q_1$. □

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Description of my own contribution

My supervisor in working on this thesis is Rupert L. Frank. The result on the three dimensional liquid drop model has been published in [13] as joint work with Rupert L. Frank and Tobias König. The result on the two dimensional liquid drop model started as joint work with Florian Behr. However, I continued working on it without him.

The three dimensional liquid drop model Rupert L. Frank posed the problem. I mostly solved the upper bound in case the minimizer is a ball. Tobias König proved most of the localization of the Perimeter in the lower bound. Apart from this it really was joint work of Tobias König and myself since we were both PhD students of Rupert Frank working in the same office. So we discussed it and solved it together. An earlier version of this paper was much more difficult since it used the sliding technique introduced by Conlon, Lieb and Yau in 1988. However, I found a shortcut that simplified the proof of the lower bound so much that this technique is not needed anymore.

Tobias König did not use this work on the liquid drop model as part of his own thesis.

The two dimensional liquid drop model This project started as joined work with Florian Behr. I worked on the upper bound and Florian Behr worked on developing the sliding method of Conlon, Lieb and Yau [11] in two dimensions. However, the shortcut that I found for the proof of the lower bound of the energy in three dimensions also works in two dimensions. This is why the work on the sliding method in two dimensions became obsolete. I continued working on the project without him. I am grateful though for his idea to use the modified Bessel function of second kind of order 0.

Eidesstattliche Versicherung

Hiermit versichere ich an Eides statt, dass ich die vorgelegte Dissertation selbstständig und ohne unerlaubte Hilfsmittel angefertigt habe.

München, den 9. Dezember 2024 Lukas Emmert

Erklärung

Hiermit erkäre ich,

- dass die Dissertation von Prof. Dr. Rupert Frank betreut wurde.
- dass bei der sprachlichen Abfassung der Dissertation keine Hilfe geleistet wurde.
- dass die Dissertation keiner anderen Prüfungskommission vorgelegen hat.
- dass ich mich nicht anderweitig einer Doktorprüfung ohne Erfolg unterzogen habe.

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